

The Flavor and Fragrance High Production Volume Consortia

The C₆-C₁₀ Consortium

Robust Summaries for C₆-C₁₀ Aliphatic Aldehydes and Carboxylic Acids

Heptanal	CAS No. 111-71-7
Heptanoic acid	CAS No. 111-14-8
Octanal	CAS No. 124-13-0
Nonanal	CAS No. 124-19-6

FFHPVC C₆-C₁₀ Aliphatic Aldehydes and Carboxylic Acids Consortium Registration Number 1101124

**Submitted to the EPA under the HPV Challenge Program by:
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Consortia**

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The evaluation of the quality of the following data uses a systematic approach described by Klimisch [Klimisch *et al.*, 1996]. Based on criteria relating to international testing standards for categorizing data reliability, four reliability categories have been established. The following categories are:

- Reliability code 1. Reliable without restrictions
- Reliability code 2. Reliable with restrictions
- Reliability code 3. Not reliable
- Reliability code 4. Not assignable

1 Chemical and Physical Properties

1.1 Melting Point

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Measured
Remarks for Test Conditions	No test conditions provided.
Melting Point	-8 °C
Remarks for Results	The data are considered reliable.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Arctander S. (1969) Perfume and Flavor Chemicals (Aroma Chemicals) II. Published Montclair, NJ.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Measured
Remarks for Test Conditions	No test conditions provided.

Melting Point	-45 °C
Remarks for Results	The data are considered reliable.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Brabec M. (1993) Aldehydes and Acetals in Patty's Industrial Hygiene and Toxicology 4th Ed., edited by G. Clayton and F. Clayton p. 286 John Wiley and Sons, Inc. New York, NY.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Measured
Remarks for Test Conditions	No test conditions provided.
Melting Point	-43.7 °C
Remarks for Results	The data are considered reliable.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Burdock G. (1995) Fenaroli's Handbook of Flavor Ingredients. Volume II, 3rd Ed. P 312, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Measured
Remarks for Test Conditions	No test conditions provided.
Melting Point	-7.5 °C
Remarks for Results	The data are considered reliable.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Burdock G. (1995) Fenaroli's Handbook of Flavor Ingredients. Volume II, 3rd Ed. P 314, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Measured
Remarks for Test Conditions	No test conditions provided.
Melting Point	-7.5 °C
Remarks for Results	The data are considered reliable.

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Merck & Co., Inc. The Merck Index (1997) 12th Edition, Publishers: Merck Research Laboratories, Whitehouse Station, NJ.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Measured
Remarks for Test Conditions	No test conditions provided.
Melting Point	-43.3 °C
Remarks for Results	The data are considered reliable.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Merck & Co., Inc. The Merck Index (1997) 12th Edition, Publishers: Merck Research Laboratories, Whitehouse Station, NJ.

Substance Name	Heptanal (data is for structurally related homologue pentanal)
CAS No.	111-71-7
Method/guideline	Measured
Remarks for Test Conditions	No test conditions provided.
Melting Point	-91.5 °C
Remarks for Results	The data are considered reliable.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Hodgman C., Weast, R. C. and Selby, S. M. (1960) Tables for identification of organic compounds Supplement to Handbook of Chemistry and Physics. Published by Chemical Rubber Publishing Co. Cleveland, Ohio.

1.2 Boiling Point

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Measured
Boiling Point	153 °C

Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Arctander S. (1969) Perfume and Flavor Chemicals (Aroma Chemicals) II. Published by the Author, Montclair, NJ.

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Measured
Boiling Point	170 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Arctander S. (1969) Perfume and Flavor Chemicals (Aroma Chemicals) II. Published by the Author, Montclair, NJ.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Measured
Boiling Point	223 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Arctander S. (1969) Perfume and Flavor Chemicals (Aroma Chemicals) II. Published by the Author, Montclair, NJ.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Measured
Boiling Point	191 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Arctander S. (1969) Perfume and Flavor Chemicals (Aroma Chemicals) II. Published by the Author, Montclair, NJ.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Measured
Boiling Point	153 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Food Chemical Codex (1996) 4th Ed., National Academy Press, Washington, D.C.

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Measured
Boiling Point	171 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Food Chemical Codex (1996) 4th Ed., National Academy Press, Washington, D.C.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Measured
Boiling Point	93 °C
Pressure	23 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Food Chemical Codex (1996) 4th Ed., National Academy Press, Washington, D.C.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Measured
Boiling Point	152.6 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Burdock G. (1995) Fenaroli's Handbook of Flavor Ingredients. Volume II, 3rd Ed., CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Measured

Boiling Point	171- 173 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Burdock G. (1995) Fenaroli's Handbook of Flavor Ingredients. Volume II, 3rd Ed., CRC Press, Boca Raton, Fl.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Measured
Boiling Point	223 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Burdock G. (1995) Fenaroli's Handbook of Flavor Ingredients. Volume II, 3rd Ed., CRC Press, Boca Raton, Fl.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Measured
Boiling Point	115 - 116 °C
Pressure	11 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Burdock G. (1995) Fenaroli's Handbook of Flavor Ingredients. Volume II, 3rd Ed., CRC Press, Boca Raton, Fl.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Measured
Boiling Point	191 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Burdock G. (1995) Fenaroli's Handbook of Flavor Ingredients. Volume II, 3rd Ed., CRC Press, Boca Raton, Fl.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Measured
Boiling Point	154 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Brabec M. (1993) Aldehydes and Acetals in Patty's Industrial Hygiene and Toxicology 4th Ed., Published by John Wiley and Sons, Inc. New York, NY.

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Measured
Boiling Point	163.4 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg

Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Merck & Co., Inc. The Merck Index (1997) 12th Ed., Publishers: Merck Research Laboratories, Whitehouse Station, NJ.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Measured
Boiling Point	152.8 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Merck & Co., Inc. The Merck Index (1997) 12th Ed., Publishers: Merck Research Laboratories, Whitehouse Station, NJ.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Measured
Boiling Point	223 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Hodgman C., Weast, R. C. and Selby, S. M. (1960) Tables for identification of organic compounds, Supplement to Handbook of Chemistry and Physics. Published by Chemical Rubber Publishing Co., Cleveland, Ohio.

Substance Name	Heptanal (data on homologous aldehydes of carbon chain length of C5-C10)
CAS No.	111-71-7
Method/guideline	Measured
Boiling Point	103.4 (pentanal) °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Hodgman C., Weast, R. C. and Selby, S. M. (1960) Tables for identification of organic compounds, Supplement to Handbook of Chemistry and Physics. Published by Chemical Rubber Publishing Co., Cleveland, Ohio.

Substance Name	Heptanal (data on homologous aldehydes of carbon chain length of C5-C10)
CAS No.	111-71-7
Method/guideline	Measured
Boiling Point	131 (hexanal) °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Hodgman C., Weast, R. C. and Selby, S. M. (1960) Tables for identification of organic compounds, Supplement to Handbook of Chemistry and Physics. Published by Chemical Rubber Publishing Co., Cleveland, Ohio.

Substance Name	Nonanal (data on homologous aldehydes of carbon chain length of C5-C10)
CAS No.	124-19-6
Method/guideline	Measured

Boiling Point	207-209 (decanal) °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Hodgman C., Weast, R. C. and Selby, S. M. (1960) Tables for identification of organic compounds, Supplement to Handbook of Chemistry and Physics. Published by Chemical Rubber Publishing Co., Cleveland, Ohio.

Substance Name	Heptanoic acid (data on structurally related acid, hexanoic acid)
CAS No.	111-14-8
Method/guideline	Measured
Boiling Point	205.5 (hexanoic acid) °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Hodgman C., Weast, R. C. and Selby, S. M. (1960) Tables for identification of organic compounds, Supplement to Handbook of Chemistry and Physics. Published by Chemical Rubber Publishing Co., Cleveland, Ohio.

Substance Name	Heptanoic acid (data on structurally related acid, octanoic acid)
CAS No.	111-14-8
Method/guideline	Measured
Boiling Point	239.3 (octanoic acid) °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.

Remarks for Reliabilities	The data are considered reliable.
References	Hodgman C., Weast, R. C. and Selby, S. M. (1960) Tables for identification of organic compounds, Supplement to Handbook of Chemistry and Physics. Published by Chemical Rubber Publishing Co., Cleveland, Ohio.

1.3 Vapor Pressure

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Calculated
Vapor Pressure	0.053 kPa (0.4 mm Hg)
Temperature	20 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are considered reliable.
References	Fragrance Materials Association (FMA)

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	MPBPWIN calculation
Vapor Pressure	0.47 kPa (3.5 mm Hg)
Temperature	25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	MPBPWIN

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	MPBPWIN calculation
Vapor Pressure	0.015 kPa (0.11 mm Hg)
Temperature	25 °C

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	MPBPWIN

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	MPBPWIN calculation
Vapor Pressure	0.21 kPa (1.6 mm Hg)
Temperature	25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	MPBPWIN

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Method/guideline	MPBPWIN calculation
Vapor Pressure	0.006 kPa (0.045 mm Hg)
Temperature	25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	MPBPWIN

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	MPBPWIN calculation
Vapor Pressure	0.075 kPa (0.56 mm Hg)
Temperature	25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.

References

MPBPWIN

Substance Name	Nonanoic acid
CAS No.	112-05-0
Method/guideline	MPBPWIN calculation
Vapor Pressure	0.0003 kPa (0.0022 mm Hg)
Temperature	25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	MPBPWIN

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	No test conditions provided.
Vapor Pressure	0.40 kPa (3 mm Hg)
Temperature	25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Data in tabular form published in standard reference text.
References	Brabec M. (1993) Aldehydes and Acetals in Patty's Industrial Hygiene and Toxicology 4th Ed., John Wiley and Sons, Inc. New York, NY.

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Calculated
Vapor Pressure	0.080 kPa (0.6 mm Hg)
Temperature	20 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are considered reliable.
References	Fragrance Materials Association (FMA)

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Calculated
Vapor Pressure	0.001 kPa (0.008 mm Hg)
Temperature	20 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are considered reliable.
References	Fragrance Materials Association (FMA)

1.4 Octanol/Water Partition Coefficients

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	KOWWIN
Log Pow	2.29
Data Qualities Reliabilities	Reliability Code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	Syracuse Research Corporation (SRC) Private communication to FMA.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	KOWWIN
Log Pow	2.42
Data Qualities Reliabilities	Reliability Code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	Syracuse Research Corporation (SRC) Private communication to FMA.

Substance Name	Octanal
CAS No.	124-13-0

Method/guideline	KOWWIN
Log Pow	2.78
Data Qualities Reliabilities	Reliability Code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	Syracuse Research Corporation (SRC) Private communication to FMA.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	KOWWIN
Log Pow	3.27
Data Qualities Reliabilities	Reliability Code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	Syracuse Research Corporation (SRC) Private communication to FMA.

Substance Name	Heptanal
CAS No.	118-58-1
Method/guideline	C-QSAR, Biobyte Corp.
Year	1994
Log Pow	2.42
Remarks for Results	Data presented in tabular form. Value consistent with log P values for 10 other linear aliphatic aldehydes.
Data Qualities Reliabilities	Reliability Code 2. Reliable with restrictions.
Remarks for Data Reliability	Data appeared in a peer-reviewed journal and are consistent with other model data.
References	Nishimura H., Saito S., Kishida F., and Matsuo, M. (1994) Analysis of acute toxicity (LD50 values) of organic chemicals to mammals by solubility parameter (delta). Acute oral toxicity to rats. Japan Journal of Industrial Health 36, 314-323.

Substance Name	Nonanal (data for structural homologue, decanal)
CAS No.	124-19-6
Method/guideline	C-QSAR, Biobyte Corp.
Year	1994

Log Pow	4.01
Remarks for Results	Data presented in tabular form. Value consistent with log P values for 10 other linear aliphatic aldehydes.
Data Qualities Reliabilities	Reliability Code 2. Reliable with restrictions.
Remarks for Data Reliability	Data appeared in a peer-reviewed journal and are consistent with other model data.
References	Nishimura H., Saito S., Kishida F., and Matsuo, M. (1994) Analysis of acute toxicity (LD50 values) of organic chemicals to mammals by solubility parameter (delta). Acute oral toxicity to rats. Japan Journal of Industrial Health 36, 314-323.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	n-Octanol/Water Partition Coefficient/Reverse Phase HPLC Method
Year	1983
Remarks for Test Conditions	The test material (1/mg/mL) in a mobile phase of methanol/water (3:1) was applied at a flow rate of 1 ml/min to a reverse phase C18-coated silica gel column fitted with a UV detector. Retention time was used to determine log Pow.
Log Pow	2.8
Remarks for Results	Measure at pH=6.7
Conclusion Remarks	HPLC Pow=2.8 and fragment-addition method Pow=2.4. Results indicate a low potential for bioaccumulation of heptanal from water.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Eadsforth C. V. (1983) Heptanal: Determination of n-octanol/water partition coefficient using a reverse-phase HPLC method. Shell Research Limited, Sittingbourne Research Centre. SBRG.83.112. Unpublished report.

1.5 Water Solubility

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	WSKOWWIN calculation
Value (mg/L) at Temperature	2274 mg/L at 25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.

References

WSKOWWIN

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	WSKOWWIN calculation
Value (mg/L) at Temperature	5316 mg/L at 25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	WSKOWWIN

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	WSKOWWIN calculation
Value (mg/L) at Temperature	715 mg/L at 25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	WSKOWWIN

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	WSKOWWIN calculation
Value (mg/L) at Temperature	132 mg/L at 25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	WSKOWWIN

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Method was not described.

Value (mg/L) at Temperature	242 at 15 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are considered reliable.
References	Merck & Co., Inc. The Merck Index (1997) Published by Merck Research Laboratories, 12th ed., Whitehouse Station, NJ.

2 Environmental Fate and Pathways

2.1 Photodegradation

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Calculation
Test Type	AOPWIN
Half-life t_{1/2}	4.2 hrs
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	AOPWIN

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Calculation
Test Type	AOPWIN
Half-life t_{1/2}	18.5 hrs
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	AOPWIN

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Calculation
Test Type	AOPWIN
Half-life t_{1/2}	4.1 hrs
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.

References

AOPWIN

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Method/guideline	Calculation
Test Type	AOPWIN
Half-life t_{1/2}	15.4 hrs
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	AOPWIN

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Calculation
Test Type	AOPWIN
Half-life t_{1/2}	3.9 hrs
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	AOPWIN

Substance Name	Nonanoic acid
CAS No.	112-05-0
Method/guideline	Calculation
Test Type	AOPWIN
Half-life t_{1/2}	13.2 hrs
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	AOPWIN

2.2 Stability in Water

Substance Name	Heptanal - No hydrolysis possible
CAS No.	111-71-7
Method/guideline	HENRYWIN
Test Type	SAR model
Half-life t_{1/2}	Volatilization half-lives of 5.9 hours from model river, and 5.1 days from model lake.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	HENRYWIN

Substance Name	Heptanoic acid - No hydrolysis possible
CAS No.	111-14-8
Method/guideline	HENRYWIN
Test Type	SAR model
Half-life t_{1/2}	Volatilization half-lives of 25 days from model river, and 189 days from model lake.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	HENRYWIN

Substance Name	Octanal - No hydrolysis possible
CAS No.	124-13-0
Method/guideline	HENRYWIN
Test Type	SAR model
Half-life t_{1/2}	Volatilization half-lives of 5.4 hours from model river, and 5.1 days from model lake.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	HENRYWIN

Substance Name	Heptanoic acid (data for homologue, octanoic acid) - No hydrolysis possible
CAS No.	124-07-2
Method/guideline	HENRYWIN
Test Type	SAR model
Half-life t_{1/2}	Volatilization half-lives of 19 days from model river, and 141 days from model lake.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	HENRYWIN

Substance Name	Nonanal - No hydrolysis possible
CAS No.	124-19-6
Method/guideline	HENRYWIN
Test Type	SAR model
Half-life t_{1/2}	Volatilization half-lives of 5.0 hours from model river, and 5.2 days from model lake.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	HENRYWIN

Substance Name	Nonanoic acid - No hydrolysis possible
CAS No.	112-05-0
Method/guideline	HENRYWIN
Test Type	SAR model
Half-life t_{1/2}	Volatilization half-lives of 14 days from model river, and 106 days from model lake.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	HENRYWIN

2.3 Biodegradation

Substance Name	Nonanal (data for structurally related homologue, decanal)
CAS No.	124-19-6
Method/guideline	The sealed vessel test is a CO ₂ production test based on OECD Guideline 301 B(1).
Test Type	Sealed Vessel Test
GLP	Yes
Year	1995
Contact Time	28 days
Innoculum	Secondary effluent from an unacclimatized activated sludge plant at URL North.
Remarks for Test Conditions	The test is conducted in a 160 ml vessel containing 100 ml mineral salt medium inoculated with secondary effluent and the respective test or reference material. The sealed vessels are incubated at 17-20 C on a rotary shaker for 28 days.
Degradation % After Time	49.8% after 28 days
Results	49.8% (95% confidence interval 41.1-58.5%)
10 day Window Criteria	No
Conclusion Remarks	The test material was not ultimately biodegradable.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was conducted in accordance with GLP and OECD guidelines.
Reference	Quest International Ltd. (1995) Biodegradability test of decanal in a sealed vessel test. Private communication to RIFM.

Substance Name	Nonanal (data for metabolite, nonanoic acid)
CAS No.	124-19-6
Method/guideline	Sealed vessel test: Modified Sturm test
Test Type	OECD 301B CO ₂ evolution
GLP	Yes
Year	1999
Contact Time	28 days
Innoculum	Nonanoic acid was added to two vessels containing mineral salts inoculated with activated sludge (10 mg C/L)

Remarks for Test Conditions	Test concentration: 10 mg/l organic carbon. Test temp: 20-24C
Degradation % After Time	72% at 29 days
Results	Nonanoic acid achieved 10% degradation by Day 2, 60% by Day 10, and 72% on Day 29.
Time required for 10% degradation	2 days
10 day Window Criteria	Yes
Total degradation	No
Conclusion Remarks	The test substance achieved the 60% pass level by Day 10. Nonanoic acid can, therefore, be considered to be readily biodegradable.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was conducted in accordance with OECD 301B guidelines.
Reference	Comb H. (1999) Pelargonic acid- Assessment of ready biodegradability- modified Sturm test. CSD 025/992285. Unpublished report to FFHPVC.

Substance Name	Nonanal (98.5% pure)
CAS No.	124-19-6
Method/guideline	Manometric Respirometry Test/OECD Guideline Method No. 302C (1981)
Test Type	OECD 302C CO ₂ evolution/O ₂ replacement
GLP	Yes
Year	1998
Contact Time	28 days
Innoculum	A known concentration of nonanal (30 mg/L) is stirred with fresh activated sludge from a waste water treatment plant in a closed flask for up to 28 days at 25 C.
Remarks for Test Conditions	The amount of O ₂ taken up during biodegradation measured as % of theoretical oxygen demand was determined by measuring the quantity of O ₂ required to maintain constant volume in the respirometer flask. Sodium benzoate (100 mg/L) was the reference substance.
Degradation % After Time	84% after 28 days
Results	Nonanal achieved 72% degradation by day 3 and 84% on day 29
Time required for 10% degradation	<1 days
10 day Window Criteria	Yes
Total degradation	No
Conclusion Remarks	The test substance (70%) achieved the 60% pass level by day 10. Nonanal can be considered to be inherently biodegradable.

Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	The study was conducted in accordance with OECD 302C guidelines.
Reference	Rudio J. (1998a) Inherent biodegradability of Aldehyde C9 Nonylic according to OECD Guideline No. 302C. Unpublished report to FFHPVC.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	The sealed vessel test is a CO2 production test based on OECD Guideline 301 B
Test Type	OECD 301 B Modified Sturm Test
GLP	Yes
Year	1984
Contact Time	28 days
Innoculum	Secondary effluent from an unacclimatized activated sludge plant from Canterbury Sewage Works
Remarks for Test Conditions	Duplicate tests were conducted in a Sturm vessel inoculated with secondary effluent and the respective test (20 mg/L) or reference material (sodium benzoate, 20 mg/L). Total CO2 evolved was measured on days 2, 4, 11, 17, 23, and 28 days.
Degradation % After Time	74 and 53% after 28 days
Results	64 and 45 % degradation after 11 days. 74 and 53% after 28 days (heptanal). 88 and 50% degradation after 28 days (sodium benzoate)
Time required for 10% degradation	2 days
10 day Window Criteria	Yes
Conclusion Remarks	The test material and standard were readily biodegradable.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was conducted in accordance with GLP and OECD guideline.
Reference	Watkinson R. J. (1984) Heptanal: An assessment of ready biodegradability. SBGR 002. Shell Research Limited, Sittingbourne Research Centre. Unpublished report.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Closed Bottle Test/OECD test guideline 301D
Test Type	301D measured as % O2 demand

GLP	Yes
Year	1984
Contact Time	28 days
Innoculum	Secondary effluent from an unacclimatized activated sludge plant from Canterbury Sewage Works was incubated with 2 mg/L heptanal or 3 mg/L standard (sodium benzoate) for 28 days at 20.1 C. O2 concentration was measured on 0, 1, 15, and 28 days.
Degradation % After Time	63 and 74% after 28 days
Results	Biodegradability measured as % theoretical O2 demand: heptanal 63 and 74%; sodium benzoate, 61 and 69%
Time required for 10% degradation	<1 day
10 day Window Criteria	Yes
Conclusion Remarks	Heptanal and standard showed >50% biodegradation after 5 days
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	The study was conducted in accordance with OECD 301D guidelines.
Reference	Watkinson R. J. (1984) Heptanal: An assessment of ready biodegradability. SBGR 002. Shell Research Limited, Sittingbourne Research Centre. Unpublished report.

Substance Name	Nonanal (97%)
CAS No.	124-19-6
Method/guideline	Manometric Respirometry Test/OECD Guideline Method No. 302C (1981)
Test Type	OECD 302C CO2 evolution/O2 replacement
GLP	Yes
Year	1994
Contact Time	28 days
Innoculum	A known concentration of nonanal (100 mg/L) is stirred with fresh activated sludge (100 mg/L) from a waste water treatment plant in a closed flask for up to 28 days at 22 C.
Remarks for Test Conditions	The amount of O2 taken up during biodegradation measured as % of theoretical oxygen demand was determined by measuring the quantity of O2 required to maintain constant volume in the respirometer flask. Sodium benzoate (100 mg/L) was the reference substance.
Degradation % After Time	32% after 28 days
Results	Nonanal achieved 29% degradation by Day 3 and 32% on Day 29. The reference material aniline was 40% degraded after 7 days and 65% after 14 days. The test material with and without

	aniline was not toxic to the microorganisms at the test concentrations.
Time required for 10% degradation	1-2days
10 day Window Criteria	No
Total degradation	No
Conclusion Remarks	The test substance undergoes 29% biodegradation by Day 10 and 32% by Day 28 Nonanal should not be regarded as readily biodegradable in this test.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	The study was conducted in accordance with OECD 301F guidelines.
Reference	Rudio J. (1998b) Ready biodegradability of Aldehyde C9 Nonylic according to OECD Guideline No. 301F. Unpublished report to FFHPVC.

2.4 Fugacity

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Air-Water Partition Coefficient
Absorption coefficient	0.0094
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
Substance Name	Heptanal

CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Soil-Water Partition Coefficient
Absorption coefficient	2.6
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	5.2
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	16.2
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Fish-Water Partition Coefficient
Absorption coefficient	6.6
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.

References

Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	12900
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Air
Estimated distribution and Media Concentration	80.8%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.

Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Water
Estimated distribution and Media Concentration	17.2%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Soil

Estimated distribution and Media Concentration	2.0%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Sediment
Estimated distribution and Media Concentration	0.045%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I

Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Suspended Sediment
Estimated distribution and Media Concentration	0.0014%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Fish
Estimated distribution and Media Concentration	0.00011%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model

Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Aerosol
Estimated distribution and Media Concentration	.000021%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Air-Water Partition Coefficient
Absorption coefficient	0.00015
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8

Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Soil-Water Partition Coefficient
Absorption coefficient	5.18
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	10.4
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	32.4
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Fish-Water Partition Coefficient
Absorption coefficient	13.2
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D.

(1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	400000
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Air
Estimated Distribution and Media Concentration	5.64%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or

References

metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Water
Estimated Distribution and Media Concentration	76.2%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Soil
Estimated Distribution and Media Concentration	17.7%

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Sediment
Estimated Distribution and Media Concentration	0.39%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP

Media	Suspended Sediment
Estimated Distribution and Media Concentration	0.012%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Fish
Estimated Distribution and Media Concentration	0.001%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay

Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Aerosol
Estimated Distribution and Media Concentration	0.00045%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Air-Water Partition Coefficient
Absorption coefficient	0.015
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs

Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Soil-Water Partition Coefficient
Absorption coefficient	8.8
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Sediment-Water Partition Coefficient
Absorption coefficient	17.6
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
Substance Name	Octanal

CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	54.9
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Fish-Water Partition Coefficient
Absorption coefficient	22.3
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	28800
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Air
Estimated Distribution and Media Concentration	84.3%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.

References

Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Water
Estimated Distribution and Media Concentration	11.2%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Soil
Estimated Distribution and Media Concentration	4.43%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.

Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Sediment
Estimated Distribution and Media Concentration	0.098%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Suspended Sediment

Estimated Distribution and Media Concentration	0.0031%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Fish
Estimated Distribution and Media Concentration	0.00025%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I

Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Aerosol
Estimated Distribution and Media Concentration	0.000049%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Air-Water Partition Coefficient
Absorption coefficient	0.00035
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model

Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Soil-Water Partition Coefficient
Absorption coefficient	16.4
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Sediment-Water Partition Coefficient
Absorption coefficient	32.7
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2

Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	102
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Fish-Water Partition Coefficient
Absorption coefficient	41.6
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	952000
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Air
Estimated Distribution and Media Concentration	13.5%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D.

(1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Water
Estimated Distribution and Media Concentration	49.3%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Soil
Estimated Distribution and Media Concentration	36.3%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or

References

metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Sediment
Estimated Distribution and Media Concentration	0.81%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Suspended Sediment
Estimated Distribution and Media Concentration	0.025%

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Fish
Estimated Distribution and Media Concentration	0.0021%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility

Media	Aerosol
Estimated Distribution and Media Concentration	0.00026%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Air-Water Partition Coefficient
Absorption coefficient	0.033
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay

Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Soil-Water Partition Coefficient
Absorption coefficient	36.6
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Sediment-Water Partition Coefficient
Absorption coefficient	73.3
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs

Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	229
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Fish-Water Partition Coefficient
Absorption coefficient	93.1
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
Substance Name	Nonanal

CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	80000
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Air
Estimated Distribution and Media Concentration	85.8%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Water
Estimated Distribution and Media Concentration	5.27%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Soil
Estimated Distribution and Media Concentration	8.68%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.

References

Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Sediment
Estimated Distribution and Media Concentration	0.19%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Suspended Sediment
Estimated Distribution and Media Concentration	0.0060%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.

Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Fish
Estimated Distribution and Media Concentration	0.00049%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Aerosol

Estimated Distribution and Media Concentration	0.00014%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Air-Water Partition Coefficient
Absorption coefficient	0.000036
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I

Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Soil-Water Partition Coefficient
Absorption coefficient	51.8
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	104
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model

Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	324
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Fish-Water Partition Coefficient
Absorption coefficient	132
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0

Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	18000000
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Air
Estimated Distribution and Media Concentration	0.54%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Water
Estimated Distribution and Media Concentration	29.4%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Soil
Estimated Distribution and Media Concentration	68.5%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D.

(1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Sediment
Estimated Distribution and Media Concentration	1.52%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Suspended Sediment
Estimated Distribution and Media Concentration	0.048%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or

References

metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Fish
Estimated Distribution and Media Concentration	0.0039%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Aerosol
Estimated Distribution and Media Concentration	0.00039%

Data Qualities Reliabilities

Reliability code 2. Reliable with restrictions.

Remarks for Data Reliability

The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.

References

Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

3 Ecotoxicity

3.1 Acute Toxicity to Fish

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Experimental: data calculated by logit transform.
Test Type	14 day LC50
GLP	No
Year	1988
Species/Strain/Supplier	P. reticulata, lab-reared
Analytical Monitoring	Gas chromatography
Exposure Period	14 days
Remarks for Test Conditions	Semi-static assay with 10 fish/concentration. Fish were acclimated to water for 12 days prior to experiment. Control fish were exposed to 72 uL/L acetone as a carrier solvent for the aldehydes. Oxygen content, pH, and concentration of test compound tested 4 times immediately before beginning of experiment and then after each renewal of test solution. Fish were fed daily. Water concentrations measured by gas chromatography. LC50s corrected for loss by evaporation.
Observations	Not reported
Conclusion Remarks	14-Day log LC50 = 1.89 umoles/L or 77.6 umoles/L or 8.85 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Complete detail on all test conditions. Data on 17 aliphatic aldehydes showed excellent correlation between log Kow and log LC50 (14-day).
Reference	Deneer J.W., Steinen, W. and Hermans, J.L.M. (1988) The acute toxicity of aldehydes to the guppy. Aquatic Toxicology, 12, 185-192.

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Experimental: data calculated by logit transform.
Test Type	14 day LC50
GLP	No

Year	1995
Species/Strain/Supplier	<i>P. reticulata</i> , lab-reared
Analytical Monitoring	Gas chromatography
Exposure Period	14 days
Remarks for Test Conditions	Semi-static assay with 10 fish/concentration. Fish were acclimated to water for 12 days prior to the experiment. Control fish were exposed to 72 uL/L acetone as a carrier solvent for the aldehydes. Oxygen content, pH, and concentration of test compound tested four times immediately before beginning of the experiment and then after each renewal of test solution. Fish were fed daily. Water concentrations were measured by gas chromatography. LC50s corrected for loss by evaporation.
Observations	Not reported
Conclusion Remarks	Acute toxicity (14 day LC50) = 1.79 umoles/L or 61.7 umoles/L or 7.89 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	Complete detail on all test conditions. Data on 17 aliphatic aldehydes showed excellent correlation between log Kow and log LC50 (14-day).
Reference	Deneer J.W., Steinen, W. and Hermans, J.L.M. (1988). The acute toxicity of aldehydes to the guppy. <i>Aquatic Toxicology</i> , 12, 185-192.

Substance Name	Heptanal (data for metabolic precursor, 1-heptanol)
CAS No.	111-71-7
Method/guideline	Calculated LC50, continuous flow-through system
Test Type	96 hr LC50
GLP	NG
Year	1995
Species/Strain/Supplier	Juvenile fathead minnows (<i>Pimephales promelas</i>)
Analytical Monitoring	HPLC and GC
Exposure Period	96 hrs
Remarks for Test Conditions	96 hour LC50 tests were performed with 26-34 day old juvenile fathead minnows. Test protocol was a continuous flow-through system according to Broderius and Kahl, 1985. Tests were carried out at 4 or 5 concentration. No solvent was required in these tests. One control (in duplicate) was used.
Observations	Not reported
Conclusion Remarks	96 hr LC50 = 37.9 mg/L

Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	US EPA Laboratory Study
Reference	Broderius S.J., Kahl, M.D. and Hoglund, M.D. (1995). Use of joint toxic response to define the primary mode of toxic action for diverse industrial organic chemicals. Environmental Toxicology and Chemistry, 14(9), 1591-1605.

Substance Name	Heptanal (data for metabolic precursor, 1-heptanol dissolved in water)
CAS No.	111-71-7
Method/guideline	Calculated LC50/Static System
Test Type	96 hr LC50
GLP	NG
Year	1984
Species/Strain/Supplier	Bleak (Alburnus alburnus), caught in Baltic Sea
Analytical Monitoring	Not reported
Exposure Period	96 hrs
Remarks for Test Conditions	Wild-caught bleak were kept at least two weeks in storage tanks with a continuous flow of natural brackish water. Bleak were fed daily until one day prior to test. All tests were performed under static conditions with no aeration of the test aquaria. Tests were performed at 6 concentrations with 1 control group. Experiments were performed in duplicate with 10 bleak per aquarium at each concentration.
Observations on Precipitation	Not reported
Conclusion Remarks	96 hr LC50 = 45 mg/L (95% CI, 42-49 mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	Methodology described in detail and results were recorded in tabular form.
Reference	Bengtsson B. E., Renberg, L. and Tarkpea, M. (1984). Molecular structure and aquatic toxicity - an example with C1-C13 aliphatic alcohols. Chemosphere, 13(5/6), 613-622.

Substance Name	Octanal (data for metabolic precursor, 1-octanol dissolved in water/acetone)
CAS No.	124-13-0
Method/guideline	Calculated LC50/Static System
Test Type	96 hr LC50
GLP	NG

Year	1984
Species/Strain/Supplier	Bleak (<i>Alburnus alburnus</i>), caught in Baltic Sea
Analytical Monitoring	Not reported
Exposure Period	96 hrs
Remarks for Test Conditions	Wild-caught bleak were kept at least two weeks in storage tanks with a continuous flow of natural brackish water. Bleak were fed daily until one day prior to test. All tests were performed under static conditions with no aeration of the test aquaria. Tests were performed at 6 concentrations with 1 control group. Experiments were performed in duplicate with 10 bleak per aquarium at each concentration.
Observations on Precipitation	Not reported
Conclusion Remarks	96 hr LC50 = 16 mg/L (95% CI, 15-17 mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	Methodology described in detail and results were recorded in tabular form.
Reference	Bengtsson B. E., Renberg, L. and Tarkpea, M. (1984). Molecular structure and aquatic toxicity - an example with C1-C13 aliphatic alcohols. <i>Chemosphere</i> , 13(5/6), 613-622.

Substance Name	Octanal (data for metabolic precursor, 1-octanol)
CAS No.	124-13-0
Method/guideline	Calculated LC50/Continuous flow-through system
Test Type	96 hr LC50
GLP	NG
Year	1984
Species/Strain/Supplier	Juvenile fathead minnows (<i>Pimephales promelas</i>)
Analytical Monitoring	HPLC and GC
Exposure Period	96 hrs
Remarks for Test Conditions	96 hour LC50 tests were performed with 26-34 day old juvenile fathead minnows. Test protocol was a continuous flow-through system. Tests were carried out at 4 or 5 concentration. No solvent was required in these tests. One control (in duplicate) was used.
Observations on Precipitation	Not reported
Conclusion Remarks	96 hr LC50 = 13.5 mg/L
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.

Data Reliability Remarks	US EPA Laboratory Study
Reference	Broderius S.J., Kahl, M.D. and. Hoglund, M.D (1995) Use of joint toxic response to define the primary mode of toxic action for diverse industrial organic chemicals. Environmental Toxicology and Chemistry, 14(9), 1591-1605

Substance Name	Heptanal (data for metabolic precursor, 1-heptanol dissolved in water)
CAS No.	111-71-7
Method/guideline	Calculated LC50/Static System
Test Type	96 hr LC50
GLP	NG
Year	1984
Species/Strain/Supplier	Nitocra spinipes (laboratory cultures)
Analytical Monitoring	Not reported
Exposure Period	96 hrs
Remarks for Test Conditions	Experiment was performed under static conditions. Nitocra spinipes were harvested from 3-6 week-old laboratory cultures; 2 times 10 harpacticoids were exposed to each concentration (at least 6 concentrations) in standard laboratory test tubes containing natural brackish water.
Observations on Precipitation	Not reported
Conclusion Remarks	96 hr LC50 = 210 mg/L (95% CI, 170-250 mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	Methodology described in detail and results were recorded in tabular form.
Reference	Bengtsson B. E., Renberg, L. and Tarkpea, M. (1984) Molecular structure and aquatic toxicity - an example with C1-C13 aliphatic alcohols. Chemosphere, 13(5/6), 613-622.

Substance Name	Nonanal (data for metabolic precursor, 1-nonanol)
CAS No.	124-19-6
Method/guideline	Calculated LC50/Continuous flow-through system
Test Type	96 hr LC50
GLP	NG
Year	1995
Species/Strain/Supplier	Juvenile fathead minnows (Pimephales promelas)

Analytical Monitoring	HPLC and GC
Exposure Period	96 hrs
Remarks for Test Conditions	96 hour LC50 tests were performed with 26-34 day old juvenile fathead minnows. Test protocol was a continuous flow-through system. Tests were carried out at 4 or 5 concentration. No solvent was required in these tests. One control (in duplicate) was used.
Observations on Precipitation	Not reported
Conclusion Remarks	96 hr LC50 = 5.52 mg/L
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	US EPA Laboratory Study
Reference	Broderius S.J., Kahl, M.D. and Hoglund, M.D. (1995) Use of joint toxic response to define the primary mode of toxic action for diverse industrial organic chemicals. Environmental Toxicology and Chemistry, 14(9), 1591-1605.

Substance Name	Octanal (data for metabolic precursor, 1-octanol dissolved in acetone/water)
CAS No.	124-13-0
Method/guideline	Calculated LC50/Static System
Test Type	96 hr LC50
GLP	NG
Year	1984
Species/Strain/Supplier	Nitocra spinipes (laboratory cultures)
Analytical Monitoring	Not reported
Exposure Period	96 hrs
Remarks for Test Conditions	Experiment was performed under static conditions. Nitocra spinipes were harvested from 3-6 week-old laboratory cultures; 2 times 10 harpacticoids were exposed to each concentration (at least 6 concentrations) in standard laboratory test tubes containing natural brackish water.
Observations on Precipitation	Not reported
Conclusion Remarks	96 hr LC50 = 58 mg/L (95% CI 53-64 mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	Methodology described in detail and results were recorded in tabular form.
Reference	Bengtsson B. E., Renberg, L. and Tarkpea, M. (1984) Molecular structure and aquatic toxicity - an example with C1-C13 aliphatic alcohols. Chemosphere, 13(5/6), 613-622.

Substance Name	Nonanal (data for metabolic precursor, 1-nonanol dissolved in acetone/water)
CAS No.	124-19-6
Method/guideline	Calculated LC50/Static System
Test Type	96 hr LC50
GLP	NG
Year	1984
Species/Strain/Supplier	Nitocra spinipes (laboratory cultures)
Analytical Monitoring	Not reported
Exposure Period	96 hrs
Remarks for Test Conditions	Experiment was performed under static conditions. Nitocra spinipes were harvested from 3-6 week-old laboratory cultures; 2 times 10 harpacticoids were exposed to each concentration (at least 6 concentrations) in standard laboratory test tubes containing natural brackish water.
Observations on Precipitation	Not reported
Conclusion Remarks	96 hr LC50 = 25 mg/L (95% CI, 21-30mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	Methodology described in detail and results were recorded in tabular form.
Reference	Bengtsson B. E., Renberg, L. and Tarkpea, M. (1984). Molecular structure and aquatic toxicity - an example with C1-C13 aliphatic alcohols. Chemosphere, 13(5/6), 613-622.

Substance Name	Nonanal (data for metabolic precursor, 1-nonanol dissolved in water/acetone)
CAS No.	124-19-6
Method/guideline	Calculated LC50/Static System Test
Test Type	96 hr LC50
GLP	NG
Year	1984
Species/Strain/Supplier	Bleak (Alburnus alburnus), caught in Baltic Sea
Analytical Monitoring	Not reported
Exposure Period	96 hrs
Remarks for Test Conditions	Wild-caught bleak were kept at least two weeks in storage tanks with a continuous flow of natural brackish water. Bleak

Observations on Precipitation	were fed daily until one-day prior to test. All tests were performed under static conditions with no aeration of the test aquaria. Tests were performed at 6 concentrations with 1 control group. Experiments were performed in duplicate with 10 bleak per aquarium at each concentration.
Conclusion Remarks	Not reported
Data Qualities Reliabilities	96 hr LC50 = 18 mg/L (95% CI, 16-20 mg/L)
Data Reliability Remarks	Reliability code 2. Reliable with restrictions.
Reference	Methodology described in detail and results were recorded in tabular form.
	Bengtsson B. E., L. Renberg and M. Tarkpea (1984). Molecular structure and aquatic toxicity - an example with C1-C13 aliphatic alcohols. Chemosphere, 13(5/6), 613-622.

Substance Name	Nonanal (data for homologous aldehyde, decanal)
CAS No.	124-19-6
Method/guideline	Experimental: data calculated by logit transform.
Test Type	14 day LC50
GLP	No
Year	1988
Species/Strain/Supplier	P. reticulata, lab-reared
Analytical Monitoring	Gas chromatography
Exposure Period	14 days
Remarks for Test Conditions	Semi-static assay with 10 fish/concentration. Fish were acclimated to water for 12 days prior to experiment. Control fish exposed to 72 uL/L acetone as a carrier solvent for the aldehydes. Oxygen content, pH, and concentration of test compound tested four times immediately before beginning of experiment and then after each renewal of test solution. Fish were fed daily. Water concentrations measured by gas chromatography. LC50s corrected for loss by evaporation.
Observations on Precipitation	Not reported
Conclusion Remarks	Acute toxicity (14 day LC50) = 1.31 umoles/L or 20.4 umoles/L or 3.10 mg/L. Note: 14-day LC50 data for octanal and decanal were determined to be 7.89 and 3.10 mg/L. It is anticipated that the 14-day LC50 is in the range of 3.10 to 7.89 mg/L.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	Complete detail on all test conditions. Data on 17 aliphatic aldehydes showed excellent correlation between logKow and log LC50 (14-day).
Reference	Deneer J.W., Steinen, W. and Hermans, J.L.M. (1988) Acute toxicity of aldehydes to the guppy. Aqua. Tox. 12, 185-192.

Substance Name	Heptanoic acid (98.7%)
CAS No.	111-14-8
Method/guideline	Calculated LC50/Semi-static system
Test Type	96 hr LC50
GLP	Yes (OECD Guideline 203)
Year	1999
Species/Strain/Supplier	Juvenile fathead minnows/Aquatic Res. Organisms
Analytical Monitoring	HPLC
Exposure Period	96 hrs
Remarks for Test Conditions	96 hour LC50 tests were performed with 26-34 day old juvenile fathead minnows. Solutions were renewed daily during the 96 hour test period. Tests were performed at a nominal concentration of 120 mg/l. The mean measured concentration was 92 mg/L.
Observations on Precipitation	Not reported
Nominal concentrations as mg/L	120 mg/L
Measured concentrations as mg/L	92 mg/L
Remarks For Results	No mortalities or sub-lethal effects were throughout the exposure period. Mean measured concentrations were 98% at 0 hours, 96 and 97% at 24 and 72 hours, respectively and 33% at 92hours. The decrease in concentration at 92 hours was reported to be due to bacterial degradation of the test article.
Conclusion Remarks	96 hr LC50 > 92 mg/L
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	OECD Guideline 203 Study
Reference	Bell G. (1999) Heptanoic acid. Acute toxicity to fathead minnows (<i>Pimephales promelas</i>). Report No. CSD 017/992696. Unpublished report to FFHPVC.

Substance Name	Heptanal (98%, methyl hexanoate, 1%)
CAS No.	111-71-7
Method/guideline	Calculated LC50/Semi-static system
Test Type	96 hr LC50
GLP	No

Year	1982
Species/Strain/Supplier	<i>Salmo gairdneri</i> fingerlings/Itchen Valley Farm
Exposure Period	96 hrs
Remarks for Test Conditions	96 hour LC50 tests were performed with 10-day-old rainbow trout. Solutions were renewed daily. Groups of ten were exposed to 0, 1, 3, 10, 30, or 100 mg/L of heptanal. All groups received 0.5 ml acetone/L. Mortality was measured every 24 hours. The temperature during test was 15.1+/-1 C, pH=8.3+/-0.2, Dissolved oxygen=10.1+/-0.2 mg/L.
Nominal concentrations as mg/L	0, 1, 3, 10, 30, 100 mg/L
Remarks For Results	Mortality at 96 hours: 0 mg/L, 0/10; 1 mg/L, 0/10; 3 mg/L, 0/10; 10 mg/L, 1/10; 30 mg/L, 10/10; 100 mg/L, 10/10
Conclusion Remarks	96 hr LC50=12 mg/L(by log/probit method)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Reference	Stephenson R. R. (1982) Heptanal: Acute toxicity to salmo gairdneri, daphnia magna, and Selenastrum capricornutum. SBGR.82.197. Shell Research Limited, Sittinbourne Research Centre. Unpublished report.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	ECOSAR
Test Type	Calculated
Species/Strain/Supplier	Fish
Exposure Period	96 hrs
Conclusion Remarks	LC50 = 8.8 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	ECOSAR
Test Type	Calculated
Species/Strain/Supplier	Fish

Exposure Period	96 hrs
Conclusion Remarks	LC50 = 389 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	ECOSAR
Test Type	Calculated
Species/Strain/Supplier	Fish
Exposure Period	96 hrs
Conclusion Remarks	LC50 = 6.7 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	ECOSAR
Test Type	Calculated
Species/Strain/Supplier	Fish
Exposure Period	96 hrs
Conclusion Remarks	LC50 = 4.8 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

3.2 Acute Toxicity to Aquatic Invertebrates

Substance Name	Heptanal (98%, methyl hexanoate, 1%)
CAS No.	111-71-7
Method/guideline	48-Hour Static Toxicity Test
GLP	No
Year	1982
Species/Strain/Supplier	Daphnia magna
Unit	mg/L
Nominal concentrations as mg/L	0, 1, 2, 5, 10, 20, 50, 100, 200 mg/L
Endpoint basis	Groups of 10 D. magna, less than 24 hours old, were allocated to a dish containing the heptanal conc. of 1.0 to 200 mg/L. All dishes received 0.5 ml acetone/L. At 24 and 48 hrs, the number of immobilized D magna were counted.
Biological observations	Immobilization test. D. magna were considered immobile, if after stirring they did not swim in 10 seconds.
EC50, EL50, LC0, at 24,48 hours	EC50 at 24 and 48 hours
Control response satisfactory?	Yes
Remarks for Test Conditions	Experiments were performed in triplicate at temperature of 20+/- 1 C, pH=8.0+/-0.2, hardness=210+/-20 mg/L as CaCO3, and dissolved oxygen=+9.1+/-0.1 mg/L.
Statistical evaluations	log/probit method
Remarks for Results	No immobilization at 0, 1, 2, or 5 mg/L. Cumulative total immobilised at 48 hours: 10 mg/L, 1/30; 20 mg/L, 3/30; 50 mg/L, 17/30; 100 mg/L, 20/30; 200 mg/L, 28/30. At 24 hours 200 mg/L, 10/30.
Conclusion Remarks	The 24 hr EC50>200 mg/L and 48 hr EC50=54 mg/L (95% C.I., 43-69 mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Reference	Stephenson R. R. (1982) Heptanal:Acute toxicity to salmo gairdneri, daphnia magna, and Selenastrum capricornutum. SBGR.82.197. Shell Research Limited, Sittinbourne Research Centre. Unpublished Report.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Daphnid

Conclusion Remarks	LC50 48 hr = 6.7 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Daphnid
Conclusion Remarks	LC50 48 hr = 429 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Daphnid
Conclusion Remarks	LC50 48 hr = 5.2 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Octanal (data for oxidation metabolite, octanoic acid)
CAS No.	124-07-2
Method/guideline	ECOSAR
Test Type	Calculation

Species/Strain/Supplier	Daphnid
Conclusion Remarks	LC50 48 hr = 167 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Daphnid
Conclusion Remarks	LC50 48 hr = 4.8 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Nonanal (data for oxidation metabolite, nonanoic acid)
CAS No.	124-19-6
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Daphnid
Conclusion Remarks	LC50 48 hr = 64 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

3.3 Acute Toxicity to Aquatic Plants

Substance Name	Heptanal (98%, methyl hexanoate, 1%)
CAS No.	111-71-7
Method/guideline	96-Hour EC50 Growth Inhibition Assay
GLP	No
Year	1982
Species/Strain/Supplier	<i>S. capricornutum</i> /ATCC 22662/American Type Culture
Unit	mg/L
Nominal concentrations as mg/L	0, 0.1, 0.2, 0.5, 1.0, 2.0, 5.0, 10, 20, and 50 mg/
Exposure period	96 hours
Endpoint basis	50% reduction in mean relative growth rate
Biological observations	Mean relative growth rate determined as the difference in log of number of cells at 48 and 96 hours/48 hours. EC50 value (conc. resulting in a 50% reduction in relative growth rate) determined by probit analysis.
Control response satisfactory?	Yes
Remarks for Test Conditions	In a 96-hr growth experiment, flasks containing 9 concentrations of heptanal were inoculated with <i>S. capricornutum</i> (500 cells/ml). Flasks were incubated in an orbital incubator at 24 C for 4 days. At 48 and 96 hrs cells were counted.
Statistical evaluations	Yes (probit analysis using log concentrations)
Conclusion Remarks	EC50 = 16 mg/L (95% C.I., 9.8-31 mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions
Reference	Stephenson R. R. (1982) Heptanal: Acute toxicity to <i>salmo gairdneri</i> , <i>daphnia magna</i> , and <i>Selenastrum capricornutum</i> . SBGR.82.197. Shell Research Limited, Sittingbourne Research Centre. Unpublished report.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Green algae

Exposure Period	96 hrs
Conclusion Remarks	EC50 = 44 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Green algae
Exposure Period	96 hrs
Conclusion Remarks	EC50 = 429 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Green algae
Exposure Period	96 hrs
Conclusion Remarks	EC50 = 17 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Octanal (data for oxidation metabolite, octanoic acid)
CAS No.	124-07-2
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Green algae
Exposure Period	96 hrs
Conclusion Remarks	EC50 = 110 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Green algae
Exposure Period	96 hrs
Conclusion Remarks	EC50 = 5.3 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Nonanal (data for oxidation metabolite, nonanoic acid)
CAS No.	112-05-0
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Green algae
Exposure Period	96 hrs

Conclusion Remarks	EC50 = 44 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

4 Human Health Toxicity

4.1 Acute Toxicity

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Method/guideline	Oral LD50/calculated Litchfield and Wilcoxon, 1949
Test Type	Oral LD50
GLP	No
Year	1964
Species/strain	Rat/Osborne-Mendel
Sex	Male and Female
# of animals per sex per dose	10
Vehicle	No vehicle required
Route of Administration	Oral
Remarks for Test Conditions	Rats fasted for 18 hours prior to treatment. All doses were given by intubation and animals were observed for an additional 14 days.
Value LD50 or LC50 with confidence limits	Oral LD50 = 10,080 (8190-12370) (95% C.I.)
Number of deaths at each dose level	Death time reported at 4 hours to 9 days.
Remarks for Results	Clinical signs included depression and diarrhea.
Conclusion Remarks	Acute oral LD50 = 10080 (8190-12370) (95% C.I.)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Jenner P.M., E. C. Hagan, J.M. Taylor, E.L. Cook and O.G. Fitzhugh (1964) Food flavourings and compounds of related structure. I. Acute oral toxicity. Food Cosmetic. Toxicology. 2:327-343.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Oral LD50
Test Type	Oral LD50

GLP	No
Year	1974
Species/strain	Rat
Sex	Not reported
# of animals per sex per dose	10
Vehicle	None reported
Route of Administration	Oral
Remarks for Test Conditions	Animals given single oral dose of 5 g/kg and observed for 14 days.
Value LD50 or LC50 with confidence limits	LD50 > 5000 mg/kg (no confidence limits reported)
Number of deaths at each dose level	No deaths reported.
Remarks for Results	Clinical signs reported included lethargy and piloerection.
Conclusion Remarks	Oral LD50 > 5000 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	Single dose to 10 animals.
References	Moreno O.M. (1974) Acute toxicity studies. Unpublished report to RIFM.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Oral LD50
Test Type	Oral LD50
GLP	No
Year	1971
Species/strain	Rat/Sherman-Wistar albino
Sex	Male and Female
# of animals per sex per dose	5
Vehicle	Not reported
Route of Administration	Oral (gavage)
Remarks for Test Conditions	Animals were fasted for 24 hours, then given single dose of 5 g/kg bw by gavage. Animals were given food and water ad libidum during a 14-day observation.

Value LD50 or LC50 with confidence limits	LD50 > 5000 mg/kg
Number of deaths at each dose level	No deaths reported.
Remarks for Results	Diuresis noted soon after dosing followed by lethargy and dullness. Recovery was complete 24-48 hr after dosing.
Conclusion Remarks	Oral LD50 > 5000 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	Single dose to 10 animals.
References	Shelanski, M.V. (1971) Acute toxicity studies in rats. Unpublished report to RIFM.

Substance Name	Octanal (mixed isomers)
CAS No.	124-13-0
Method/guideline	Oral LD50
Test Type	Oral LD50
GLP	No
Year	1962
Species/strain	Rat/Wistar
Sex	Male
# of animals per sex per dose	5
Vehicle	Not specified
Route of Administration	Oral (gavage)
Remarks for Test Conditions	Five non-fasted male rats were used in this study. Chemicals administered undiluted (if possible) or diluted in water, corn oil or 1% TERGITOL via gastro-intubation.
Value LD50 or LC50 with confidence limits	5.63 mL/kg or 4616 mg/kg
Number of deaths at each dose level	No specifics reported.
Remarks for Results	No range was calculable because no dosage resulted in fractional mortality.
Conclusion Remarks	Oral LD50 = 5.63 mL/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	No details regarding doses and mortality.
References	Smyth Jr., H.F., C. P. Carpenter, C.S. Weil, U.C. Pozzani and J.A. Striegel (1962) Range finding toxicity data: List VI. Industrial Hygiene Assn. J. 23: 95-107.

Substance Name	Heptanoic acid (data for homologue, octanoic acid) (mixed isomers)
CAS No.	124-07-2
Method/guideline	Oral LD50
Test Type	Oral LD50
GLP	No
Year	1962
Species/strain	Rat/Wistar
Sex	Male
# of animals per sex per dose	5
Vehicle	Not specified
Route of Administration	Oral
Remarks for Test Conditions	Chemicals administered undiluted (if possible) or diluted in water, corn oil or 1% TERGITOL via gastro-intubation.
Value LD50 or LC50 with confidence limits	LD50 = 1.41 (0.88-2.29) mL/kg or 1283 mg/kg
Number of deaths at each dose level	Not reported
Conclusion Remarks	Oral LD50 = 1.41 (0.88-2.29) mL/kg or 1283 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	No details given regarding doses and mortality.
References	Smyth Jr., H.F., C. P. Carpenter, C.S, Weil, U.C. Pozzani and J.A. Striegel (1962) Range finding toxicity data: List VI. Industrial Hygiene Assn. J. 23: 95-107.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	LD50/calculated
Test Type	LD50
GLP	No
Year	1976
Species/strain	Rats/albino
Sex	Male and Female

# of animals per sex per dose	4
Vehicle	No vehicle used
Route of Administration	Oral
Value LD50 or LC50 with confidence limits	Oral LD50 = 8,370 (std. dev. +/- 1203 mg/kg)
Number of deaths at each dose level	1350 mg/kg, 0/4; 4556 mg/kg, 0/4; 6834 mg/kg, 1/4; 10,250 mg/kg, 3/4; 15,380 mg/kg, 4/4
Remarks for Results	Symptoms increasing in duration and severity with dose included hypoactivity, salivation, labored breathing, muscular weakness and prostration. Necropsy of dead animals revealed hemorrhaged lungs. At 2 highest doses, animals exhibited burns to GI tract.
Conclusion Remarks	Heptanoic acid was concluded to be practically nontoxic
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions
Remarks for Data Reliability	Although a small number of animals were used at each dose, results are consistent with other oral LD50 values.
References	Harrison W.A. (1976a) Acute Oral Toxicity Studies with heptanoic acid (SN1767). Industrial Biotest Laboratories, P.O. No. 045-858-76. Private Communication to FFHPVC. Unpublished report.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Dermal LD50
Test Type	Dermal LD50
GLP	No
Year	1974
Species/strain	Rabbit
Sex	Not reported
# of animals per sex per dose	10
Vehicle	Not reported
Route of Administration	Dermal
Remarks for Test Conditions	Animals given single dermal dose of 5 g/kg.
Value LD50 or LC50 with confidence limits	LD50 > 5000 mg/kg (no confidence limits reported)
Number of deaths at each dose level	No deaths reported
Remarks for Results	Symptoms reported include skin irritation: moderate redness (8/10), marked redness (2/10), moderate edema (7/10), and marked edema (3/10).

Conclusion Remarks	Dermal LD50=>5000 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	Single dose to 10 animals.
References	Moreno O.M. (1974) Acute toxicity studies. Unpublished report to RIFM.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Method/guideline	Dermal LD50
Test Type	Dermal LD50
GLP	No
Year	1977
Species/strain	Rabbit
Sex	Not reported
# of animals per sex per dose	10
Vehicle	Not reported
Route of Administration	Dermal
Value LD50 or LC50 with confidence limits	LD50 > 5000 mg/kg
Number of deaths at each dose level	No deaths were described.
Remarks for Results	Clinical signs and observations included; 0/10 mortality, diarrhea in 1/10 on day 11, skin irritation; 10/10 reported to have severe redness, 10/10 reported to have moderate edema.
Conclusion Remarks	Dermal LD50 > 5000 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	Single dose to 10 animals.
References	Moreno O.M. (1977) Acute toxicity studies. Unpublished report to RIFM.

Substance Name	Octanal (mixed isomers)
CAS No.	124-13-0
Method/guideline	Occluded 24 hr patch (Draize et al., 1944)
Test Type	Dermal LD50

GLP	No
Year	1962
Species/strain	Rabbit/albino New Zealand
Sex	Male
# of animals per sex per dose	4
Vehicle	Not reported
Route of Administration	Dermal
Remarks for Test Conditions	Fur was removed from entire trunk. The dose was applied beneath an impervious plastic. Animals immobilized during the 24-hour contact period after which the film was removed and the rabbits caged for the subsequent 14-day period.
Value LD50 or LC50 with confidence limits	LD50 = 6.35 mL/kg (4.70-8.59) or 5207 mg/kg
Number of deaths at each dose level	Not described
Remarks for Results	Based on mortalities during a 14-day observation period, the most probable LD50 value and its fiducial range are estimated by the method of Thompson (1947) using the tables of Weil (1952).
Conclusion Remarks	Dermal LD50 = 6.35 mL/kg (4.70-8.59) or 5207 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	No detail regarding doses and mortality.
References	Smyth Jr., H.F., C. P. Carpenter, C.S, Weil, U.C. Pozzani and J.A. Striegel (1962) Range finding toxicity data: List VI. Industrial Hygiene Assn. J. 23: 95-107.

Substance Name	Heptanoic acid (data for homologue, octanoic acid) (mixed isomers)
CAS No.	124-07-2
Method/guideline	Occluded 24 hr Patch (Draize et al., 1944)
Test Type	Dermal LD50
GLP	No
Year	1962
Species/strain	Rabbit/albino New Zealand
Sex	Male
# of animals per sex per dose	4
Vehicle	Not reported

Route of Administration	Dermal
Remarks for Test Conditions	Fur was removed from entire trunk. The dose was applied beneath an impervious plastic. Animals immobilized during the 24-hour contact period after which the film was removed and the rabbits caged for the subsequent 14-day period.
Value LD50 or LC50 with confidence limits	Dermal LD50 = 0.71 mL/kg or 647 mg/kg
Number of deaths at each dose level	Not described
Remarks for Results	No range was calculable because no dosage resulted in fractional mortality.
Conclusion Remarks	Dermal LD50 = 0.71 mL/kg or 647 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	No details given regarding doses and mortality.
References	Smyth Jr., H.F., C. P. Carpenter, C.S, Weil, U.C. Pozzani and J.A. Striegel (1962) Range finding toxicity data: List VI. Industrial Hygiene Assn. J. 23: 95-107.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Dermal LD50
Test Type	Dermal LD50
GLP	No
Year	1971
Species/strain	Rabbit/albino
Sex	Not reported
# of animals per sex per dose	6
Vehicle	Not reported
Route of Administration	Dermal
Remarks for Test Conditions	Single dermal dose of 5 g/kg; applied on 3 rabbits with intact skin and 3 rabbits with abraded skin.
Value LD50 or LC50 with confidence limits	LD50 > 5000mg/kg
Number of deaths at each dose level	One death recorded on day 4.
Remarks for Results	Severe edema and burns at site of application.
Conclusion Remarks	Acute dermal LD50 = >5000 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.

References

Shelanski M.V. (1971) Acute toxicity studies in rats.
Unpublished report to RIFM.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Dermal LD50
Test Type	LD50
GLP	No
Year	1976
Species/strain	Rabbits/albino
Sex	Male and Female
# of animals per sex per dose	4
Vehicle	No vehicle used
Route of Administration	Dermal
Value LD50 or LC50 with confidence limits	LD50 = >2000 mg/kg
Number of deaths at each dose level	2000 mg/kg, 1(M)/4
Remarks for Test Conditions	The material was applied undiluted to the abraded skin of 2 male and 2 female rabbits.
Remarks for Results	Body weights were reduced over the 14 day observation period. Skin changes at 24 hours included severe erythema, edema, and second and third degree burns. Necrosis was reported at skin sites at 14 days.
Conclusion Remarks	Heptanoic acid was concluded to be practically nontoxic
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions
Remarks for Data Reliability	Results are consistent with other oral LD50 values.
References	Harrison W.A. (1976b) Acute Dermal Toxicity Studies with heptanoic acid (SN1767). Industrial Biotest laboratories, P.O. No. 045-858-76. Private Communication to FFHPVC. Unpublished report.

Substance Name	Nonanal (data for nonanoic acid, 97%)
CAS No.	124-19-6
Method/guideline	Inhalation LC50
Test Type	Inhalation LC50
GLP	EPA GLP 40 CFR 792 (TSCA)

Year	1990
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
# of animals per sex per dose	10 (5M & 5F)
Vehicle	None
Route of Administration	Inhalation
Remarks for Test Conditions	Groups of Sprague-Dawley rats (5/sex) were exposed to aerosols containing a concentration of 0.046 or 3.8 mg/L of nonanoic acid for 4 hours. Exposure levels and particle size were measured 4 times. Animals were held for 14 day post-exposure.
Value LD50 or LC50 with confidence limits	LC50 between 0.46 and 3.8 mg/L (mean gravimetric exposure conc.) with a nominal concentration of 0.60 and 31 mg/L, respectively.
Number of deaths at each dose level	Eight (8) animals died at 3.8 mg/L. There were no mortalities at 0.46 mg/L.
Remarks for Results	Signs of irritation were noted during exposure and the first week post-exposure. Survivor's recovery within 14 days. Particle size distribution measurements showed average mass median diameter of 2.9 to 3.6 microns with 92% of the aerosol <10 microns.
Conclusion Remarks	The acute LC50 for nonanoic acid in male and female rats is > 0.46 mg/L but <3.8 mg/L.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Hoffman G. (1990) Acute inhalation toxicity study of nonanoic acid in the rat. Project No. 89-8216. Unpublished report to FFHPVC.

Substance Name	Heptanoic acid (98.5%)
CAS No.	111-14-8
Method/guideline	Inhalation LC50
Test Type	Inhalation LC50
GLP	EPA GLP 40 CFR 792 (TSCA)
Year	1990
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
# of animals per sex per dose	10 (5M & 5F)
Vehicle	None
Route of Administration	Inhalation

Remarks for Test Conditions	Groups of Sprague-Dawley rats (5/sex) were exposed to an aerosol containing a target concentration of 5.0 mg/L of heptanoic acid for 4 hours. Exposure levels and particle size were measured 4 times. Animals were held for 14 day post-exposure.
Value LD50 or LC50 with confidence limits	LC50 > 4.6 mg/L (mean gravimetric exposure conc.) with a nominal concentration of 28 mg/L.
Number of deaths at each dose level	Four animals died
Remarks for Results	Signs of irritation were noted during exposure and for several days post-exposure. Survivor's recovery within 14 days. Particle size distribution measurements showed average mass median diameter of 3.8 microns with 92% of the aerosol < 10 microns.
Conclusion Remarks	LC50 > 4.6mg/L for male and female rats
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Hoffman G. (1990) Acute inhalation toxicity study of heptanoic acid in the rat. Project No. 89-8215. Unpublished report to FFHPVC.

Substance Name	Heptanal (90.8%)
CAS No.	111-71-7
Method/guideline	Inhalation LC50
Test Type	Inhalation LC50
GLP	EPA GLP 40 CFR 792 (TSCA)
Year	1989
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
# of animals per sex per dose	6 (3M & 3F)
Vehicle	None
Route of Administration	Inhalation
Remarks for Test Conditions	Groups of Sprague-Dawley rats (3/sex) were exposed to an atmosphere containing a target concentration of 5.0 mg/L of heptanal for 4 hours. Animals were observed at 15-minute intervals during the first hour exposure and daily post exposure.
Value LD50 or LC50 with confidence limits	LC50 > 4.7 mg/L (average exposure concentration)
Number of deaths at each dose level	No deaths recorded.
Remarks for Results	Nominal exposure concentration was 5.9 mg/L and average particle size was 0.80 mg/m ³ .
Conclusion Remarks	LC50 > 4.7mg/L for male and female rats

Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Berardi, M.R. (1989) Acute inhalation toxicity study of heptanal in the rat. Project No. 88-8086. Unpublished report to FFHPVC.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Method/guideline	LD50/calculated per Miller and Tainter (1944).
Test Type	LD50
GLP	No
Year	1961
Species/strain	Mouse (strain not specified)
Sex	Male and Female
# of animals per sex per dose	6 groups of 10 mice per material
Vehicle	2% emulsion w cottonseed oil
Route of Administration	Injection (tail vein)
Value LD50 or LC50 with confidence limits	LD50 = 600 +/- 24 mg/kg
Number of deaths at each dose level	Not reported
Conclusion Remarks	Acute injected LD50 = 600 +/- 24 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	Incomplete data on doses and strain.
References	Oro K. and A. Wretland (1961) Pharmacological effects of fatty acids, triolein and cottonseed oil. Acta Parmacol. Et Toxicol. 18:141-152.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	LD50/calculated per Miller and Tainter (1944).
Test Type	LD50
GLP	No
Year	1961
Species/strain	Mouse (strain not specified)
Sex	Male and Female

# of animals per sex per dose	6 groups of 10 mice per material
Vehicle	5% aqueous solution-cottonseed oil
Route of Administration	Injection (tail vein)
Value LD50 or LC50 with confidence limits	LD50 = 1200 +/- 56 mg/kg
Number of deaths at each dose level	Not reported
Conclusion Remarks	Acute injected LD50 = 1200 +/- 56 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	Incomplete data (doses, strain)
References	Oro K. and A. Wretland (1961) Pharmacological effects of fatty acids, triolein and cottonseed oil. Acta Pharmacol. Et Toxicol. 18:141-152.

4.2 In vitro Genotoxicity

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse mutation assay
System of Testing	Bacterial
GLP	Yes
Year	1992
Species/Strain	Salmonella typhimurium strains TA97, TA98, TA100, TA1535, TA1537
Metabolic Activation	Aroclor 1254-induced hamster or rat liver
Doses/Concentration	1, 3, 10, 33, 100, 166, 333, 1000, 1666, 3333 ug/plate
Remarks for Test Conditions	Preincubation procedure (Haworth et al 1983), with and without metabolic activation. Substance was considered mutagenic if it produced a reproducible, dose-related response over solvent control.
Results	Negative results in all strains with and without S9.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Heptanal not mutagenic

Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	Study performed by National Toxicology Program.
References	Zeiger, E., Anderson, B., Haworth, S., Lawlor, T., and Mortelmans, K. (1992). Salmonella mutagenicity tests: V. Results from the testing of 311 chemicals. Environ Molecul Mutagenesis 19(Suppl 21): 2-141.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse mutation assay
System of Testing	Bacterial
GLP	No
Year	1980
Species/Strain	Salmonella typhimurium strains TA98, TA100, TA1535, TA1537
Metabolic Activation	S9 mix from Aroclor 1254 or methylcholanthrene-induced rats
Doses/Concentration	3 umol/plate (402 ug/plate)
Statistical Methods	Average of two experiments
Remarks for Test Conditions	Test material was dissolved in ethanol.
Results	No increase in the incidence of reverse mutations with or without S9 activation.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Heptanal was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The study lacked an adequate description of statistical methods.
References	Florin, I., L. Rutberg, M. Curvall and C.R. Enzell (1980) Screening of tobacco smoke constituents for mutagenicity using the Ames' Test. Toxicology, 18:219-232.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse mutation assay

System of Testing	Bacterial
GLP	No
Year	1980
Species/Strain	Salmonella typhimurium strains TA98, TA100, TA1535, TA1537
Metabolic Activation	S9 mix from Aroclor 1254 or methylcholanthrene-induced rats
Doses/Concentration	3 umol/plate (486 ug/plate)
Statistical Methods	Average of two experiments
Remarks for Test Conditions	Test material was dissolved in ethanol.
Results	There was no increase in the frequency of reverse mutations with or without S9 activation.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	The test material was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The study lacked an adequate description of statistical methods.
References	Florin, I., L. Rutberg, M. Curvall and C.R. Enzell (1980). Screening of tobacco smoke constituents for mutagenicity using the Ames' Test. Toxicology 18:219-232.

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse mutation assay
System of Testing	Bacterial
GLP	No
Year	1980
Species/Strain	Salmonella typhimurium strains TA98, TA100, TA1535, TA1537
Metabolic Activation	S9 mix from Aroclor 1254 or methylcholanthrene-induced rats
Doses/Concentration	3 umol/plate (444 ug/plate)
Statistical Methods	Average of two experiments
Remarks for Test Conditions	Test material was dissolved in ethanol.
Results	There was no increase in the frequency of reverse mutations with or without S9 activation.

Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	The test material was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The study lacked an adequate description of statistical methods.
References	Florin, I., L. Rutberg, M. Curvall and C.R. Enzell (1980) Screening of tobacco smoke constituents for mutagenicity using the Ames' Test. Toxicology 18:219-232.

Substance Name	Nonanal (98%)
CAS No.	124-19-6
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Salmonella preincubation assay
System of Testing	Bacterial
GLP	Yes
Year	1986
Species/Strain	Salmonella typhimurium strains TA97, TA98, TA100, TA1535, TA1537
Metabolic Activation	S9 mix from Aroclor 1254-induced Sprague-Dawley rats
Doses/Concentration	0, 1, 3.5, 10, 35, 100, 355, 666 ug/plate
Statistical Methods	Not reported
Remarks for Test Conditions	Preincubation (48hrs), concurrent solvent and positive controls were tested with and without the metabolic activation systems, 7 dose levels and 3 plates per dose. All assays were repeated no less than 1 week after completion of the initial test.
Results	No increase in reverse mutations at any dose as compared to the solvent control.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Non mutagenic in this assay
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	Study performed by National Toxicology Program.
References	Mortelmans, K., S. Haworth, T. Lawlor, W. Speck, B. Tainer and E. Zeiger (1986). Salmonella mutagenicity tests: II. Results from the testing of 270 chemicals. Environ. Mutagen. 8(Suppl7): 1-119.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Ames (preincubation procedure) (Maron and Ames, 1983)
Test Type	Reverse mutation assay
System of Testing	Bacterial
GLP	No
Year	1985
Species/Strain	Salmonella typhimurium strains TA102, TA104
Doses/Concentration	Up to 1 mg/plate (1000 ug/plate)
Statistical Methods	Not reported
Remarks for Test Conditions	Test material was dissolved in either DMSO or water, preincubation with glutathione (end of preincubation period determined by time to decrease toxicity to long-chain alkenals)
Results	Maximum non-toxic dose = 0.4 umol/plate (65 ug/plate), no increase in reverse mutations.
Cytotoxic concentration	> 0.4 umol/plate
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was reported to show no evidence of mutagenicity in this assay.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The study lacked an adequate description of statistical methods and doses.
References	Marnett, L.J., H.K. Hurd, M.C. Hollstein, D.E. Levin, H. Esterbauer and B.N. Ames (1985). Naturally occurring carbonyl compounds are mutagens in Salmonella tester strain TA104. Mutation Research 148:25-34.

Substance Name	Heptanal (data for a structurally related aldehyde, 5-heptenal, 2,6-dimethyl)
CAS No.	111-71-7
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse mutation assay
System of Testing	Bacterial
GLP	NG
Year	1983

Species/Strain	Salmonella typhimurium strains TA98, TA100, TA1535, TA1537, TA1538
Metabolic Activation	S9 liver fractions prepared from Aroclor-induced rats
Doses/Concentration	Five concentrations up to 3600 ug/plate
Statistical Methods	Kastenbaum and Bowman, 1970
Remarks for Test Conditions	Plates were incubated for 48 hours. DMSO used as a solvent for poorly soluble chemicals. Positive controls included 0.5 ug/plate of sodium azide for TA 1535 (430-760 revertants/plate) and TA 100 (400-700 revertants/plate) and 5ug/plate of benzo[a]pyrene for TA 100 (865-1210 revertants/plate), TA1537 235-350 revertants/plate), TA1538 (410-590 revertants/plate, and TA98 (660-1000 revertants/plate).
Results	No significant increased in reverse mutations.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Specific doses not reported and details of specific chemical not described. Data presented in tabular form.
References	Wild, D., M.-T. King, E. Gocke and K. Eckhardt (1983). Study of artificial flavouring substances for mutagenicity in the Salmonella /Microsome, BASC and micronucleus tests. Fd. Chem. Toxic. 21:707-719

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Ames assay (Ames et al., 1973; McCann et al., 1975)
Test Type	Reverse mutation assay
System of Testing	Bacterial
GLP	NG
Year	1989
Species/Strain	Salmonella typhimurium strains TA98, TA100, TA1535, TA1537, TA1538
Metabolic Activation	S9 fraction of Aroclor 1254-induced Sprague-Dawley rat liver
Doses/Concentration	Up to 150,000 ug/plate
Remarks for Test Conditions	Bacteria were culture in Oxford medium #2 for 12 hours. Assays were conducted by addition of 2.0 ml of test article to agar along with 0.1 ml of bacterial culture and either metabolic activation mix or an equivalent volume of phosphate buffer. The mixture was incubated for 48 hours and revertant colonies counted.

Results	No increase in reverse mutations, with or without S9 mix.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Heptanoic acid was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Heck, J.D., T.A. Vollmuth, M.A. Cifone, D.R. Jagannath, B. Myhr and R.D. Curren (1989). An evaluation of food flavoring ingredients in a genetic toxicity screening battery. The Toxicologist 9(1): 257.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Method/guideline	Ames assay (Ames et al., 1973; McCann et al., 1975)
Test Type	Reverse mutation assay
System of Testing	Bacterial
GLP	NG
Year	1989
Species/Strain	Salmonella typhimurium strains TA98, TA100, TA1535, TA1537, TA1538
Metabolic Activation	S9 fraction of Aroclor 1254-induced Sprague-Dawley rat liver
Doses/Concentration	Up to 50000 ug/plate
Remarks for Test Conditions	Bacteria were culture in Oxford medium #2 for 12 hours. Assays were conducted by addition of 2.0 ml of test article to agar along with 0.1 ml of bacterial culture and either metabolic activation mix or an equivalent volume of phosphate buffer. The mixture was incubated for 48 hours and revertant colonies counted.
Results	No increase in reverse mutations, with or without S9 mix.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Octanoic acid was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Heck, J.D., T.A. Vollmuth, M.A. Cifone, D.R. Jagannath, B. Myhr and R.D. Curren (1989). An evaluation of food flavoring ingredients in a genetic toxicity screening battery. The Toxicologist 9(1): 257.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse Mutation Assay
System of Testing	Bacterial
GLP	Yes
Year	1980
Species/Strain	Salmonella typhimurium TA1537, TA1538, TA98
Metabolic Activation	Aroclor 1254-induced hamster or rat liver
Doses/concentration levels	0.0001 to 0.01 ul/plate
Remarks for Test Conditions	A solution of the test article, positive controls or solvent control were mixed with the test organisms and applied to agar plates. The plates were then incubated at 37 °C for 48 hours. A positive mutagenesis concluded if it produced a reproducible, dose-related increase in reverse mutants is 2 to 3 times that for solvent control. Positive controls included 2-nitrofluorene for TA98 and TA1538 and 9-aminoacridine for TA1537.
Results	Negative results in all strains at all concentrations with and without S9.
Cytotoxic concentration	0.01 ul/plate
Genotoxic effects	None reported
Remarks for results	Tests using TA100 and TA1535 were discarded because of bacterial contamination.
Conclusion Remarks	Under these test conditions and according to the evaluation criteria, heptanal was not mutagenic in Salmonella typh. Stains TA 98, TA 1537, and TA1538 with or without metabolic activation.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Jagannath D.R. (1980) Mutagenic evaluation of C-191 in the Ames salmonella/microsome plate test. Project no. 20988. Unpublished report to FFHPVC.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse Mutation Assay

System of Testing	Bacterial
GLP	Yes
Year	1980
Species/Strain	Salmonella typhimurium TA1537, TA1538, TA98
Metabolic Activation	Aroclor 1254-induced hamster or rat liver
Doses/concentration levels	0.0001 to 0.01 ul/plate
Remarks for Test Conditions	A solution of the test article, positive controls or solvent control were mixed with the test organisms and applied to agar plates. The plates were then incubated at 37 C for 48 hours. A positive mutagenesis concluded, if it produced a reproducible, dose-related increase in reverse mutants is 2 to 3 times that for solvent control. Positive controls included 2-nitrofluorene for TA98 and TA1538 and 9-aminoacridine for TA1537.
Results	Negative results in all strains at all concentrations with and without S9.
Cytotoxic concentration	0.01 ul/plate for TA 1537/ TA1538; > 0.01 ul TA98
Genotoxic effects	None reported
Remarks for results	Tests using TA100 and TA1535 were discarded because of bacterial contamination.
Conclusion Remarks	Under these test conditions and according to the evaluation criteria, nonanal was not mutagenic in Salmonella typh. Stains TA 98, TA 1537, and TA1538 with or without metabolic activation.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Jagannath D.R. (1980) Mutagenic evaluation of C-192 in the Ames salmonella/microsome plate test. Project no. 20988. Unpublished report to FFHPVC.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse Mutation Assay
System of Testing	Bacterial
GLP	Yes
Year	1989
Species/Strain	Salmonella typhimurium TA100, TA1535, TA1537, TA1538, TA98
Metabolic Activation	Aroclor 1254-induced hamster or rat liver
Doses/concentration levels	Five concentrations from 667 to 10,000 ug/plate with S9 and from 100 to 5000 ug/plate without S9

Remarks for Test Conditions	A solution of the test article, positive controls or solvent (DMSO) control were mixed with the tester strain in molten agar at 45 C and applied to agar plates. The plates were then incubated at 37 C for 48 hours. A positive mutagenesis concluded, if the test article produced a reproducible, dose-related increase in mean number of reverse mutants at least 2 times that for solvent control. Positive controls included 2-aminoanthracene and 2-nitrofluorene for TA98 and 1538, 2-aminoanthracene and sodium azide for TA 100 and TA1535, 2-aminoanthracene and ICR-191 for TA1537.
Results	Negative results in all strains at all concentrations with and without S9.
Cytotoxic concentration	>10000 ug/plate +S9 and >5000 ug/plate -S9
Genotoxic effects	None reported
Conclusion Remarks	Under these test conditions and according to the evaluation criteria, there was no evidence that heptanoic acid was mutagenic in Salmonella typhimurium strains TA 98, TA 100, TA1535, TA 1537, and TA1538 with metabolic activation at concentrations up to 10000 ug/plate and without metabolic activation at concentrations up to 5000 ug/plate..
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	San R.H. and Schadly, M.B. (1989) Salmonella/microsome plate incorporation mutagenicity assay with heptanoic acid. Study no. T87768.501. Unpublished report to FFHPVC.

Substance Name	Nonanal (data for nonanoic acid)
CAS No.	124-19-6
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse Mutation Assay
System of Testing	Bacterial
GLP	Yes
Year	1989
Species/Strain	Salmonella typhimurium TA100, TA1535, TA1537, TA1538, TA98
Metabolic Activation	Aroclor 1254-induced hamster or rat liver
Doses/concentration levels	Five concentrations from 667 to 10,000 ug/plate
Remarks for Test Conditions	A solution of the test article, positive controls or solvent (DMSO) control were mixed with the tester strain in molten agar at 45 C and applied to agar plates. The plates were then incubated at 37 C for 48 hours. A positive mutagenesis concluded, if the test article produced a reproducible, dose-related increase in mean number of reverse mutants at least 2 times that for solvent control. Positive controls included 2-aminoanthracene and 2-nitrofluorene for TA98 and 1538, 2-

Results	aminoanthracene and sodium azide for TA 100 and TA1535, 2-aminoanthracene and ICR-191 for TA1537.
Cytotoxic concentration	Negative results in all strains at all concentrations with and without S9. >10000 ug/plate
Genotoxic effects	None reported
Conclusion Remarks	Under these test conditions and according to the evaluation criteria, there was no evidence that nonanoic acid was mutagenic in Salmonella typh. strains TA 98, TA 100, TA1535, TA 1537, and TA1538 with and without metabolic activation at concentrations up to 10000 ug/plate.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	San R.H. and Kruel C. (1989) Salmonella/microsome plate incorporation mutagenicity assay with pelargonic acid. Study no. T87769.501. Unpublished report to FFHPVC.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Mouse lymphoma assay (Clive et al., 1979)
Test Type	Mammalian mutation assay
System of Testing	Mouse lymphoma cell
GLP	NG
Year	1989
Species/Strain	L5178Y mouse lymphoma cell
Metabolic Activation	Induced rat liver S9 and cofactors
Doses/Concentration	900 ug/ml with S9, 600 ug/ml without S9
Remarks for Test Conditions	Thymidine kinase competent heterozygote was exposed to the test article in the presence or absence of S9. After a 4-hour exposure, cells were washed, incubated (48hrs) to allow phenotypic expression, and colonies were counted after 10-14 days growth. Mutant frequency calculated using the ratio of mutant to viable colonies cloned without selective medium.
Results	Negative at 900 ug/mL with S9 and weakly positive at 600 ug/mL without S9.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Heptanoic acid was not mutagenic in the presence of metabolic activation and weakly mutagenic without metabolic activation.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Heck, J.D., T.A. Vollmuth, M.A. Cifone, D.R. Jagannath, B. Myhr and R.D. Curren (1989). An evaluation of food flavoring

ingredients in a genetic toxicity screening battery. The Toxicologist 9(1): 257.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Mouse lymphoma assay (Clive et al., 1979)
Test Type	Mammalian Mutation Assay
System of Testing	Mouse lymphoma forward mutation assay
GLP	NG
Year	1981
Species/Strain	L5178Y mouse lymphoma cell
Metabolic Activation	Aroclor 1254 from Fisher N344 male rats
Doses/concentration levels	0.78 to 100 nl/ml without S9, 6.25 to 250 ng/ml with S9
Remarks for Test Conditions	Thymidine kinase competent heterozygote cells were exposed to the test article in the presence or absence of S9. After a 4-hour exposure, cells were washed, incubated (48-hrs) to allow phenotypic expression, and colonies were counted after 10 days growth. Mutant frequency calculated using the ratio of mutant to viable colonies cloned without selective medium.
Results	No evidence of mutagenicity concentrations up to 100 nl/ml without metabolic activation and 250 nl/ml with metabolic activation.
Cytotoxic concentration	125 nl/ml without S9, >250 nl/ml with S9
Genotoxic effects	None reported
Remarks for results	Without metabolic activation, moderate toxicity was observed at 0.78 nl/ml and high toxicity (8.8 to 5.8 % relative growth) was observed for concentrations from 50 to 100 nl/ml. With metabolic activation, weak toxicity (69.3% rel. growth) was observed at 6.25 nl/ml and moderate toxicity (22.8 % rel. growth) was observed for the 250 nl/ml concentration.
Conclusion Remarks	Concentrations up to 100 nl/ml without metabolic activation and 250 nl/ml with metabolic activation did not result in any evidence of mutagenicity in the mouse lymphoma forward mutation assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Myhr B. (1981) Mutagenic an evaluation of heptanal in the mouse lymphoma forward mutation assay. LBI Project No. 20989. Unpublished Report to FFHPVC.

Substance Name	Nonanal
CAS No.	124-19-6

Method/guideline	Mouse lymphoma assay (Clive et al., 1979)
Test Type	Mammalian Mutation Assay
System of Testing	Mouse lymphoma forward mutation assay
GLP	NG
Year	1981
Species/Strain	L5178Y mouse lymphoma cell
Metabolic Activation	Aroclor 1254 from Fisher N344 male rats
Doses/concentration levels	0.0977 to 25 nl/ml without S9, 0.0977 to 50 nl/ml with S9 (trial 1) and 6.25 to 120 nl/ml (trial 2)
Remarks for Test Conditions	Thymidine kinase competent heterozygote cells were exposed to the test article in the presence or absence of S9. After a 4-hour exposure, cells were washed, incubated (48hrs) to allow phenotypic expression, and colonies were counted after 10 days growth. Mutant frequency calculated using the ratio of mutant to viable colonies cloned without selective medium. Three repeat trials were performed without activation and two with activation.
Results	No evidence of mutagenicity at concentrations up to 25 nl/ml without metabolic activation. Weak evidence of mutagenicity with metabolic activation in trail 2 (1.9 fold increase compared to controls) at cytotoxic (24% rel. growth) concentration of 25 nl/ml and 2.2 fold increase in mutational frequency at cytotoxic levels (10-15% rel. growth) of 60 and 120 nl/ml.
Cytotoxic concentration	31.3 nl/ml without S9, >250 nl/ml with S9
Genotoxic effects	Slight increase (2.2 fold) at 60 & 120 nl/ml.
Remarks for results	Without metabolic activation, there is no evidence of toxicity even at cytotoxic levels. With metabolic activation, weak mutagenic activity is associated with high cytotoxicity concentration.
Conclusion Remarks	Concentrations up to 25 nl/ml of nonanal without metabolic activation show no evidence of mutagenicity. Cytotoxic concentration of 60 and 120 nl/ml with activation show weak evidence of mutagenicity.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Myhr B. (1981). Mutagenic an evaluation nonanal in the mouse lymphoma forward mutation assay. LBI Project No. 20989. Unpublished Report to FFHPVC.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Sister chromatid exchange (SCE)
Test Type	Cytogenetic assay

System of Testing	Rat hepatocytes
GLP	NG
Year	1993
Species/Strain	Female Fischer 344 rat hepatocytes
Doses/Concentration	0, 0.1, 1.0, 10 or 100 uM in DMSO/plate (0, 16.2, 162, 1620, or 16,200 ug/plate)
Statistical Methods	Student's t test (dependent variables)
Remarks for Test Conditions	Aldehyde solutions in DMSO were added to culture medium containing freshly prepared F344 rat hepatocytes by a collagenase perfusion technique. Isolated hepatocytes were plated at a density of 20,000 cells/plate. After 3 hours incubation medium was removed and cultures were washed twice and 5ml of medium containing insulin (10-7M). Approximately 20 hours after the exchange an aqueous solution of nonanal in DMSO (<1%) was added to the cultures to yield a final concentration of 0.1, 1.0, 10, or 100 uM. The cultures were then incubated for 3 hours. The medium was washed twice and supplemented with EGF (40 ng/ml) and bromodeoxyuridine (10 uM). 48 Hours later Colcemid (0.4 ug/ml) were added and incubated for 3 hours. For chromosomal aberrations and sister chromatid exchange analysis, the medium was replaced with 2ml collagenase (0.5 mg/ml) and the plates were incubated for an additional 10 minutes. Twenty (20) well-spread second division metaphases were scored individually, except for concentrations with a very low rate.
Results	Significant increase in SCE at 0.1 and 10 uM/plate ($p<0.05$), and at 1 and 100 uM/plate ($p<0.01$). No dose-response relationship. Data for induction of SCE (mean +/- std deviation); Control; 0.75+/-0.05; 0.1 uM, 0.95+/-0.07; 1.0 uM, 1.05+/-0.09; 10 uM, 1.13+/-0.09; 100 uM, 1.01+/-0.09.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was reported to result in cytogenetic damage in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The controls, statistics and concentrations tested were described in detail.
References	Eckl, P.M., A. Ortner and H. Esterbauer (1993). Genotoxic properties of 4-hydroxyalkenals and analogous aldehydes. Mutation Research 290:183-192.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Cytogenetic assay (Eckl et al., 1987; Michalopoulos et al., 1982)
Test Type	Chromosomal aberrations
System of Testing	Non bacterial
GLP	No
Year	1990
Species/Strain	Fischer 344 rat hepatocytes
Doses/Concentration	0, 0.1, 1.0, 10 or 100 uM/plate (0, 16.2, 162, 1620, or 16,200 ug/plate)
Statistical Methods	Student's t test (independent variables)
Remarks for Test Conditions	Aldehyde solutions (1-40 uM in 0.9% NaCl) were added to culture medium containing freshly prepared rat hepatocytes. After 3 hours incubation medium was removed and cultures were washed twice and 5ml of medium containing epidermal growth factor (40 ng/ml) and bromodeoxyuridine (10 uM) were added. 48 hours later Colcemid (0.4 ug/ml) were added and incubated for 3 hours. For chromosomal aberrations at least 20 metaphases were scored. The number of chromosomal aberrations is given per diploid cell (42 chromosomes).
Results	At 100 uM, there was an increase (32-fold) in aberrations compared to controls. The increase was not statistically significant because of the high standard deviation in the assay. Therefore, there was no statistically significant increase in chromosomal aberrations in this assay. Control; 0.015+/-0.03; 0.1 uM, 0.31+/-0.2; 1.0 uM, 0.17+/-0.35; 10 uM, 0.19+/-0.32; 100 uM, 0.49+/-0.70
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The controls, statistics and concentrations tested were described in detail.
References	Esterbauer, H., P. Eckl and A. Ortner (1990) Possible mutagens derived from lipids and lipid precursors. Mutation Research, (238), 223-233.

Substance Name	Nonanal
CAS No.	124-19-6

Method/guideline	Cytogenetic assay (Eckl et al., 1987; Michalopoulos et al., 1982)
Test Type	Micronuclei
System of Testing	Rat hepatocytes
GLP	No
Year	1990
Species/Strain	Fischer 344 rat hepatocytes
Doses/Concentration	0, 0.1, 1.0, 10 or 100 uM/plate (0, 16.2, 162, 1620, or 16,200 ug/plate)
Statistical Methods	Student's t test (dependent variables)
Remarks for Test Conditions	Aldehyde solutions (1-40 uM in 0.9% NaCl) were added to culture medium containing freshly prepared rat hepatocytes. After 3 hours incubation medium was removed and cultures were washed twice and 5ml of medium containing epidermal growth factor (40 ng/ml) and bromodeoxyuridine (10 uM) were added. 48 hours later Colcemid (0.4 ug/ml) were added and incubated for 3 hours. For micronuclei counts, cells were fixed and stained with DAPI. 1000 cells were scored to determine the % of mitotic cells and the % of cells with micronuclei.
Results	No significant increase in the frequency of micronuclei in micronucleated polychromatic erythrocytes. Data for % of cells with micronuclei (mean +/- std deviation); Control; 0.00; 0.1 uM, -1.01+/-6.19; 1.0 uM, 1.97+/-7.8; 10 uM, -3.77+/-7.5; 100 uM, 4.57+/-16.6.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was not genotoxic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The controls, statistics and concentrations tested were described in detail.
References	Esterbauer, H., P. Eckl and A. Ortner (1990). Possible mutagens derived from lipids and lipid precursors. Mutat. Res. 238:223-233.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Cytogenetic assay (Eckl et al., 1987; Michalopoulos et al., 1982)
Test Type	Mitotic index
System of Testing	Rat hepatocytes
GLP	No

Year	1990
Species/Strain	Fischer 344 rat hepatocytes
Doses/Concentration	0, 0.1, 1.0, 10 or 100 uM/plate (0, 16.2, 162, 1620, or 16,200 ug/plate)
Statistical Methods	Student's t-test (for independent variables)
Remarks for Test Conditions	Aldehyde solutions (1-40 uM in 0.9% NaCl) were added to culture medium containing freshly prepared rat hepatocytes. After 3 hours incubation medium was removed and cultures were washed twice and 5ml of medium containing epidermal growth factor (40 ng/ml) and bromodeoxyuridine (10 uM) were added. 48 hours later Colcemid (0.4 ug/ml) were added and incubated for 3 hours. For micronuclei counts, cells were fixed and stained with DAPI. 1000 Cells were scored to determine the % of mitotic cells and the % of cells with micronuclei.
Results	No significant increase in the frequency of mitotic index. Data for % of mitotic cells (mean +/- std deviation); Control; 0.41+/- 0.16; 0.1 uM, 0.44+/-0.31; 1.0 uM, 0.41+/-0.22; 10 uM, 0.46+/- 0.28; 100 uM, 0.52+/-0.37.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The controls, statistics and concentrations tested were described in detail.
References	Esterbauer, H., P. Eckl and A. Ortner (1990). Possible mutagens derived from lipids and lipid precursors. Mutation Research 238:223-233.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Cytogenetic assay
Test Type	Cytogenetic assay
System of Testing	Rat hepatocytes
GLP	NG
Year	1993
Species/Strain	Female Fischer 344 rat hepatocytes
Doses/Concentration	0, 0.1, 1.0, 10 or 100 uM in DMSO/plate (0, 16.2, 162, 1620, or 16,200 ug/plate)
Statistical Methods	Student's t test (dependent variables)

Remarks for Test Conditions	Aldehyde solutions in DMSO were added to culture medium containing freshly prepared F344 rat hepatocytes by a collagenase perfusion technique. Isolated hepatocytes were plated at a density of 20,000 cells/plate. After 3 hours incubation medium was removed and cultures were washed twice and 5ml of medium containing insulin (10-7M). Approximately 20 hours after the exchange an aqueous solution of nonanal in DMSO (<1%) was added to the cultures to yield a final concentration of 0.1, 1.0, 10, or 100 uM. The cultures were then incubated for 3 hours. The medium was washed twice and supplemented with EGF (40 ng/ml) and bromodeoxyuridine (10 uM). 48 hours later Colcemid (0.4 ug/ml) was added and incubated for 3 hours. 1000 cells were analyzed under the fluorescence microscope.
Results	No significant increase in the frequency of micronuclei in micronucleated polychromatic erythrocytes. Data for increase in frequency of micronuclei (mean +/- std deviation); Control; 12.82+/-8.4; 0.1 uM, 10.64+/-7.3; 1.0 uM, 14.8+/- 10.6; 10 uM, 7.68+/-2.36; 100 uM, 16.0+/-18.9.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Non-mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The controls, statistics and concentrations tested were described in detail.
References	Eckl, P.M., A. Ortner and H. Esterbauer (1993). Genotoxic properties of 4-hydroxyalkenals and analogous aldehydes. Mutation Research 290:183-192.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Chromosomal aberration assay
Test Type	Cytogenetic assay
System of Testing	Rat hepatocytes
GLP	NG
Year	1993
Species/Strain	Female Fischer 344 rat hepatocytes
Doses/Concentration	0, 0.1, 1.0, 10 or 100 uM in DMSO/plate (0, 16.2, 162, 1620, or 16,200 ug/plate)
Statistical Methods	Student's t test (dependent variables)
Remarks for Test Conditions	Aldehyde solutions in DMSO were added to culture medium containing freshly prepared F344 rat hepatocytes by a collagenase perfusion technique. Isolated hepatocytes were

	<p>plated at a density of 20,000 cells/plate. After 3 hours incubation medium was removed and cultures were washed twice and 5ml of medium containing insulin (10-7M). Approximately 20 hours after the exchange an aqueous solution of nonanal in DMSO (<1%) was added to the cultures to yield a final concentration of 0.1, 1.0, 10, or 100 uM. The cultures were then incubated for 3 hours. The medium was washed twice and supplemented with EGF (40 ng/ml) and bromodeoxyuridine (10 uM). 48 Hours later Colcemid (0.4 ug/ml) were added and incubated for 3 hours. For chromosomal aberrations and sister chromatid exchange analysis, the medium was replaced with 2ml collagenase (0.5 mg/ml) and the plates were incubated for an additional 10 minutes. Twenty (20) well-spread second division metaphases were scored individually, except for concentrations with a very low rate. Data collected on results of six experiments at each concentration. No increase in the incidence of chromosomal aberrations. Data for induction of chromosomal aberrations (mean +/- std deviation); Control; 0.01+/-0.03; 0.1 uM, 0.31+/-0.28; 1.0 uM, 0.17+/-0.35; 10 uM, 0.19+/-0.32; 100 uM, 0.49+/-0.70.</p>
Results	
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was not genotoxic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The controls, statistics and concentrations tested were described in detail.
References	Eckl, P.M., A. Ortner and H. Esterbauer (1993). Genotoxic properties of 4-hydroxyalkenals and analogous aldehydes. Mutation Research 290:183-192.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Unscheduled DNA synthesis (Williams, 1977)
Test Type	Unschedule DNA synthesis assay
System of Testing	Rat hepatocytes
GLP	NG
Year	1994
Species/Strain	Sprague-Dawley male albino rat hepatocytes
Doses/Concentration	0, 3, 10, 30, 100 mM
Statistical Methods	Student's t-test (two-tailed)
Remarks for Test Conditions	Cultures exposed for 20 hours to n-alkanals and 10 uCi/mL [methyl-3H]thymidine and were processed immediately after treatment for the autoradiographic evaluation of UDS.

Results	Substance was evaluated in 2 independent tests, nuclear grain counts of 200 cells. Positive and negative controls were n-dimethylnitrosoamine and solvent, respectively. No increase in unscheduled DNA synthesis.
Cytotoxic concentration	100 mM
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was not genotoxic in this assay
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Martelli, A., R. Canonero, M. Cavanna, M. Ceradelli and U. Marinari (1994) Cytotoxic and genotoxic effects of five n-alkanals in primary cultures of rat and human hepatocytes. Mutation Research, 323:121-126.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Unscheduled DNA synthesis (Williams, 1977)
Test Type	Unschedule DNA synthesis assay
System of Testing	Human hepatocytes
GLP	NG
Year	1994
Species/Strain	Human hepatocytes
Doses/Concentration	0, 3, 10, 30, 100 mM
Statistical Methods	Student's t-test (two-tailed)
Remarks for Test Conditions	Human hepatocyte suspensions were prepared from apparently healthy fragments of human liver discarded during the course of prescribed surgery (Strom et al., 1982). Cultures exposed 20 hours to n-alkanals and 10 uCi/mL [methyl-3H]thymidine and were processed immediately after treatment for the autoradiographic evaluation of UDS. Substance was evaluated in 2 independent tests, nuclear grain counts of 200 cells. Positive and negative controls were n-dimethylnitrosoamine and solvent, respectively.
Results	No increase in unscheduled DNA synthesis.
Cytotoxic concentration	100 mM
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was not genotoxic in this assay.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions

References

Martelli, A., R. Canonero, M. Cavanna, M. Ceradelli and U. Marinari (1994). Cytotoxic and genotoxic effects of five n-alkanals in primary cultures of rat and human hepatocytes. *Mutation Research* 323:121-126.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Unscheduled DNA synthesis (Williams, 1977, 1980; Buttersworth et al., 1987)
Test Type	Unschedule DNA synthesis assay
System of Testing	Rat hepatocytes
GLP	Not reported
Year	1989
Species/Strain	Fischer or Sprague-Dawley rat hepatocytes
Doses/Concentration	1000 ug/ml
Remarks for Test Conditions	Cultures were incubated for 18-20 hrs with the test article. Unscheduled DNA synthesis measured by electronically counting nuclear grains in the nucleus and in 3 adjacent nuclear-sized cytoplasmic areas, for each dose level. Either 75 or 150 cells were analyzed. Net grains counts for the nucleus and cytoplasm were recorded. Positive UDS was indicated by an increase of at least 6 net grains per nucleus as compared to the solvent control. Negative control was DMSO and positive control was 2-acetylaminofluorene (AAF).
Results	No evidence of UDS at 1000 ug/mL.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Heptanoic acid was not genotoxic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The controls and other methodology were complete.
References	Heck, J.D., T.A. Vollmuth, M.A. Cifone, D.R. Jagannath, B. Myhr and R.D. Curren (1989). An evaluation of food flavoring ingredients in a genetic toxicity screening battery. <i>The Toxicologist</i> 9(1): 257.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Method/guideline	Unscheduled DNA synthesis (Williams, 1977, 1980; Buttersworth <i>et al.</i> , 1987)

Test Type	Unschedule DNA synthesis assay
System of Testing	Rat hepatocytes
GLP	NG
Year	1989
Species/Strain	Fischer or Sprague-Dawley rat hepatocytes
Remarks for Test Conditions	Cultures were incubated for 18-20 hours with the test article. Unscheduled DNA synthesis measured by electronically counting nuclear grains in the nucleus and in 3 adjacent nuclear-sized cytoplasmic areas, for each dose level. Either 75 or 150 cells were analyzed. Net grains counts for the nucleus and cytoplasm were recorded. Positive unscheduled DNA synthesis was indicated by an increase of at least 6 net grains per nucleus as compared to the solvent control. Negative control was DMSO and positive control was 2-acetylaminofluorene (AAF).
Results	No evidence of UDS at 300 ug/mL.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Octanoic acid was not genotoxic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Heck, J.D., T.A. Vollmuth, M.A. Cifone, D.R. Jagannath, B. Myhr and R.D. Curren (1989). An evaluation of food flavoring ingredients in a genetic toxicity screening battery. The Toxicologist 9(1): 257.

4.3 In vivo Genotoxicity

Substance Name	Heptanal (data for structurally related aldehyde, 5-heptenal, 2,6-dimethyl)
CAS No.	111-71-7
Method/guideline	BASC test on Drosophila was performed as reported in Eckhardt, King, Gocke and Wild, 1980.
Test Type	BASC test (Wurgler, Sobels and Vogel, 1977)
GLP	NG
Year	1983
Species/Strain	Insect, Drosophila melanogaster
Sex	Male and Female
Route of Administration	Feed

Doses/Concentration	25 mM
Exposure Period	48 hrs
Remarks for Test Conditions	The test substance to be fed to the flies was prepared in 5% saccharose, with addition of 2% ethanol and 2% Tween 80. Ethyl nitrite was administered to Drosophila males in gaseous form. To do this, flies were kept for 3 days in 1-liter bottle containing small amount of medium, and ethyl nitrite was injected into the tightly closed bottles.
Genotoxic effects	None
NOEL (C)/ LOEL (C)	25 mM
Remarks for Results	No mutagenic activity was demonstrated under the test conditions. Data for number of sex-linked recessive lethal chromosome. Brood I 6/1847; Brood II, 6/1811; Brood III, 4/1966. Control: Brood I, 42/18188; Brood II, 34/17734; Brood III, 50/16980.
Conclusion Remarks	No mutagenic activity was demonstrated under the test conditions
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed Journal Food and Chemical Toxicology.
References	Wild, D., King, M. -T., Gocke, E. and Eckhardt, K. (1983). Study of Artificial Flavouring Substances for Mutagenicity in the Salmonella/Microsome, BASC and Micronucleus Tests. Food and Chemical Toxicology 21(6): 707-719.

Substance Name	Heptanal (data for structurally related aldehyde, 5-heptenal, 2,6-dimethyl)
CAS No.	111-71-7
Method/guideline	Micronucleus test. NMRI mice were treated once with the test material. The mice were killed and bone-marrow smear was prepared 30 hours after the treatment. The smears were stained according to the method of Schmid & the slides were scored.
Test Type	Micronucleus test
GLP	NG
Year	1983
Species/Strain	NMRI mice
Sex	Male and Female
Route of Administration	Not given
Doses/Concentration	0, 420, 980, 1540 mg/kg
Exposure Period	Single intraperitoneal injection
Remarks for Test Conditions	Test material injected into 4 mice. The vehicle was olive oil.

Effect on mitotic index or PCE/NCE ratio by dose level and sex	At 0 mg/kg, 1.7=mean MNPE/1000NPE; At 420mg/kg, 1.0=mean MNPE/1000 NPE; At 980 mg/kg 1.5=MNPE/1000 NPE; At 1540 mg/kg, 2.2= MNPE/1000 NPE NPE=Normal Polychromatic erythrocytes; MNPE=Micronucleated Polychromatic erythrocytes.
Genotoxic effects	None
NOEL (C)/ LOEL (C)	1540 mg/kg
Statistical Evaluation	Kastenbaum and Bowman, 1970.
Remarks for Results	No mutagenic activity was detected under the test conditions.
Conclusion Remarks	No mutagenic activity was detected under the test conditions.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed Journal Food and Chemical Toxicology.
References	Wild, D., King, M.-T., Gocke, E. and Eckhardt, K. (1983) Study of Artificial Flavouring Substances for Mutagenicity in the Salmonella/Microsome, BASC and Micronucleus Tests. Food and Chemical Toxicology 21(6): 707-719.

4.4 Repeat Dose Toxicity

Substance Name	Heptanal (data for structurally related aldehyde, 2,6-dimethylhept-5-en-1-al)
CAS No.	111-71-7
Method/guideline	90-day feeding study
GLP	NG
Year	1983
Species/strain	Rat/Wistar, pathogen free
Sex	Male and Female
Route of Administration	Diet
Doses/concentration Levels	0, 9, 37, 150 mg 2,6-dimethylhept-5-en-1-al/kg bw/day
Exposure Period	90 days
Frequency of Treatment	Daily
Control Group	Yes
Post Exposure Observation Period	None
Remarks for Test Conditions	After a 4-day acclimatization period, rats were divided randomly into four groups of 15 animals of each sex and maintained on

	diets to provide daily intakes of 0 (control), 10, 40 and 60 mg/kg bw/day for 13-14 weeks. Rats were examined daily for mortality and clinical signs. Rats were weighed twice weekly and food consumption was measured daily. Water intake was recorded twice weekly. Blood was collected from the retro-orbital plexus at week 6 and from the aorta of anesthetized rats at week 13/14. Hematology examined hemoglobin concentration, erythrocyte count, packed cell volume and leucocyte count. Serum clinical chemistry was performed on serum at weeks 6 and 13/14. Urine samples were collected during week 6 and during the last week of the study and examined for volume, pH, glucose, blood, bile, ketones and protein. At the end of the study, the rats were necropsied and histopathological examination of major tissues and organs (29) were performed.
NOAEL (NOEL)	37 mg/kg/bw/d
LOAEL (LOEL)	150 mg/kg/bw/d
Actual Dose Received by Dose Level and Sex	9, 36.6, 149.2 (m); 8.9, 36.5, 153.1 (f) mg/kg bw/d
Toxic Response/effects by Dose Level	At 150 mg/kg/body weight; slight decrease in renal concentrating ability was reported at week 6 in males and at week 14 in females. Serum glucose levels of both sexes were elevated as compared to the controls at 150 mg/kg bw/d. There were no evidence of histopathology to any tissue or organ including the testes and ovaries.
Statistical Evaluation	Student's t-test (99 and 95%)
Conclusion Remarks	Administration of these doses produced no marked toxic effects in the rats, treatment of the rats had no effect on body weights, food or water intake. The higher hemoglobin concentrations in treated groups were not considered to be adverse findings. The cause of the increased serum glucose level at the highest dose is unknown.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliabilities Remarks	Study was published in a peer-reviewed journal.
References	Gaunt, I.F., G. Wright, R. Cottrell and S. D. Gangolli (1983) Short-term toxicity of 2,6-dimethylhept-5-en-1-al in rats. Journal of Food and Chemical Toxicology, 21(5): 543-549.

Substance Name	Octanal (data for a mixture containing blend of aldehydes; C-8: Octanal (4 ppm), C-9: Nonanal (9 ppm), C-10 (2.2 ppm), C-11 (6 ppm), C-12 (6 ppm), C-12 (6 ppm) and methyl nonyl acetaldehyde (8 ppm)
CAS No.	124-13-0
Method/guideline	90-day feeding study
GLP	No
Year	1958
Species/strain	Rat

Sex	Male and Female
Route of Administration	Diet
Doses/concentration Levels	112 mg aliphatic aldehyde mixture/kg bw/d
Exposure Period	90 days
Frequency of Treatment	Daily
Control Group	Yes, basal diet only
Post Exposure Observation Period	None
Remarks for Test Conditions	Groups of 12 rats were maintained on diets containing 100 mg/kg bw of aldehyde mixture for 12 weeks. Controls were maintained on an unsupplemented diet. After 12 weeks, urine samples were examined for presence of sugar and albumin, and blood hemoglobin levels. At necropsy, liver and kidney weights were measured and the liver and kidneys were subjected to histopathological examination.
NOAEL (NOEL)	112 mg/kg bw/d
LOAEL (LOEL)	Not reported
Actual Dose Received by Dose Level and Sex	112 mg/kg body weight
Statistical Evaluation	Not reported
Remarks for Results	There was no effect on growth, food intake, or efficiency of food utilization. Based on hematological examination urine analysis, liver and kidney weights and histopathological examination of liver and kidney tissues, there was no evidence of toxicity associated with administration of the test substance.
Conclusion Remarks	The authors reported no adverse effects on growth, food intake, efficiency of food utilization or other physiological criteria (survival, body weight, behavior, appearance, urinalysis, blood hemoglobin, liver and kidney weights)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	Study performed under contract to Food and Drug Administration. It was part of a screening program in which limited clinical chemistry, hematology, and histopathology was performed.
References	Trubeck Laboratories (1958) Toxicological examination of blend of aliphatic aldehydes in rats. Class III, Part 2. Unpublished report.

Substance Name	Heptanal (data for structurally related aldehyde, 5-heptenal, 2,6-dimethyl)
CAS No.	111-71-7
Method/guideline	29-day oral gavage study
GLP	Yes (CFR Pt 58, 1978)

Year	1990
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
Route of Administration	Gavage
Doses/concentration Levels	0, 300, 1500, and 3000 mg/kg bw/day
Exposure Period	29 days
Frequency of Treatment	Daily
Control Group	Yes (vehicle only)
Post Exposure Observation Period	None
Remarks for Test Conditions	Groups (10/sex/group) of rats, 44 days old were given the test substance by gavage in corn oil (10 ml/kg) daily for 29 days. Clinical signs were monitored twice weekly and body weights and food consumption were measured weekly. Baseline hematology and clinical chemistry were performed on 10 animals prior to initiation of the study. These animals were then discarded. At termination, all animals were fasted overnight. The animals were injected with ketamine and blood samples were drawn for clinical chemistry and hematology. At necropsy, organ weights were measured and tissues (26) were preserved in 10% formalin. All 26 tissues from controls and high-dose groups and the heart, liver, kidneys, and gross lesions from the low- and mid-dose group were embedded in paraffin, stained with hematoxylin and eosin, and examined microscopically.
NOAEL (NOEL)	300 mg/kg bw/day
LOAEL (LOEL)	1500 mg/kg bw/day
Toxic Response/effects by Dose Level	At 3000 mg/kg, 1 male and 3 females died during treatment. Other signs included languid behavior, prostration, ataxia and excess salivation. Clinical chemistry examination revealed increased alkaline phosphatase (males), increased total protein and albumin (both sexes). Significantly increased absolute and relative liver and kidney weights were accompanied by minimal centrilobular to diffuse hepatocellular hypertrophy, decreased periportal vaculization and increased hepatocellular cytoplasm density. In the kidney, male rats exhibited increased severity of hyaline droplets. Acanthosis was reported in the non-glandular stomach. At 1500 mg/kg bw/day, dose-related increases in total protein and albumin levels and histopathology of the liver and kidney were reported. At 300 mg/kg/bw/day, there were no significant findings that could be related to administration of the test material.
Statistical Evaluation	Anova, then Dunnett's Comparison
Conclusion Remarks	Based on statistically significant changes in liver and kidney weights and histopathology of these organs 1500 mg/kg bw/day was considered the lowest observable adverse effect level (LOAEL) and 300 mg/kg bw/day was considered the no

observable adverse effect level (NOAEL)

Data Qualities Reliabilities

Reliability Code 1. Reliable without restrictions.

Data Reliabilities Remarks

Study was conducted in compliance with Good Laboratory Practice Regulations, Title 21, U. S. Code of Federal Regulations Part 58

References

Terrill J. B. (1990a) 28-Day oral toxicity study in rats with 5-heptenal, 2,6-dimethyl. Lab. Project ID 642-482. Hazelton laboratories. Unpublished Report.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	27-day oral gavage study
GLP	Yes (CFR Pt 58, 1978)
Year	1990
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
Route of Administration	Gavage
Doses/concentration Levels	0, 875, 1750, and 3500 mg/kg bw/day
Exposure Period	27 days
Frequency of Treatment	Daily
Control Group	Yes (vehicle only)
Post Exposure Observation Period	None
Remarks for Test Conditions	Groups (10/sex/group) of rats 45 days of age were given the test substance by gavage in corn oil (10 ml/kg) daily for 27 days. Clinical signs were monitored twice weekly and body weights and food consumption were measured weekly. Baseline hematology and clinical chemistry were performed on 10 animals prior to initiation of the study. These animals were then discarded. At termination, all animals were fasted overnight. The animals were injected with ketamine and blood samples were drawn for clinical chemistry and hematology. At necropsy, organ weights were measured and tissues (26) were preserved in 10% formalin. All 26 tissues from controls and high-dose groups and the heart, liver, kidneys, and gross lesions from the low- and mid-dose groups were embedded in paraffin, stained with hematoxylin and eosin, and examined microscopically.
NOAEL (NOEL)	1750 mg/kg bw/day
LOAEL (LOEL)	3500 mg/kg bw/day

Toxic Response/effects by Dose Level	At 3500 mg/kg, 1 male and 5 females died during treatment. Five of the 6 deaths were considered related to gavage administration. Other signs included languid behavior, dyspnea, polypnea, tremors, wheezing, ataxia and excess salivation. Clinical chemistry and hematological examinations revealed no significant changes compared to those for the control group. A significant decrease in body weight and food consumption (males only) were recorded compared to those of the control group. Increased relative organ weight changes were not associated with a morphological change, but reflected lower terminal body weights. At necropsy, hyperkeratosis of the non-glandular stomach was reported in high-dose males and females. The rough and thickened mucosa of the non-glandular stomach noted at necropsy suggested a mild local irritation associated with gavage administration. At 875 and 1750 mg/kg bw/day dose levels, there were no significant findings that could be related to administration of the test material.
Statistical Evaluation	Yes. ANOVA, then Dunnett's Comparison
Conclusion Remarks	Based on decreased body weights and food consumption, gross lesions of the stomach, and microscopic lesions of the non-glandular region of the stomach, the 3500 mg/kg bw/day was considered the lowest observable adverse effect level (LOAEL). The dose level of 1750 mg/kg bw/day was considered the no observable adverse effect level (NOAEL).
Data Qualities Reliabilities	Reliability Code 1. Reliable without restrictions.
Data Reliabilities Remarks	Study was conducted in compliance with GLP Regulations, Title 21, U. S. Code of Federal Regulations Part 58
References	Terrill J. B. (1990b) 28-Day oral toxicity study in rats with heptanoic acid. Lab. Project ID 642-480. Hazelton Labs. Unpublished Report.

Substance Name	Heptanal (data for homologue, hexanal, 99%)
CAS No.	111-71-7
Method/guideline	28-day drinking water study
GLP	No
Year	1988
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
Route of Administration	Drinking water
Doses/concentration Levels	0.1, 0.9, 8.6, or 95.7 mg/kg/day/1.0, 10.0, 100.0, or 1000 mg/L
Exposure Period	28 days
Frequency of Treatment	Continuously
Control Group	0.05% Emuphor in water

Post Exposure Observation Period	None
Remarks for Test Conditions	Groups of SD rats (10/sex/group) were maintained on drinking water containing 1.0, 10.0, 100.0, or 1000 mg/L of hexanal for 4 weeks. Control groups received tap water and a vehicle control group received 0.5% Emuphor. Clinical observations were made daily and body weight, food and water consumption were made weekly. At necropsy brain, heart, liver, spleen and kidneys were weighed. At termination, hematological and clinical chemistry examinations were performed. Histopathology was performed on 26 tissues in controls and the highest exposure group.
NOAEL (NOEL)	95.7 mg/kg/day
Actual Dose Received by Dose Level and Sex	0.1, 0.9, 8.6, or 95.7 mg/kg/day
Toxic Response/effects by Dose Level	Based on measurement of body weight change, food and water consumption, hematological examination of the highest dose group, clinical chemistry examination, organ weights changes, and gross and histopathological examination, there were no significant differences between any treatment group and the control groups.
Statistical evaluations?	One-way analysis of variance.
Conclusion Remarks	There were no adverse effects related to the intake of up to 95.7 mg/kg/day of hexanal in drinking water.
Remarks for Results	Sporadic observations of dilated kidney pelvis (one animal at 10 mg/L and one at 100 mg/L) and hydronephrosis (one animal at 1000 mg/L) were not dose related and were no related to administration of the test material.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The study was performed at the Environmental and Occupational Toxicology Division, Environmental Health Directorate, Canada
References	Komsta E., Chu I., Secours V. E., Valli V.E., Villeeneuve D. C. (1988) Results of a short-term toxicity study for three organic chemicals found in Niagara River drinking water. Bull. Environ. Contam. Toxicol, 41:515-522.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Mouse Skin Bioassay
GLP	Yes
Year	1985
Species/strain	Mouse C3H/HeJ
Sex	Male
Route of Administration	Dermal

Doses/concentration Levels	50 mg as a 75% solution in mineral oil
Exposure Period	80 weeks
Frequency of Treatment	Twice weekly
Control Group	Three control groups: Control group 1, no treatment; Control group 2, mineral oil; Positive control group 3, 0.05% benzo(a)pyrene in mineral oil.
Post Exposure Observation Period	None
Remarks for Test Conditions	Groups (50) of male mice were housed 5 per cage. Food and water were provided ad libitum. Mice were weighed weekly for the first month and thereafter every two weeks. Heptanoic acid (50 mg) in mineral oil, mineral oil (negative control), or 0.05% benzo(a)pyrene in mineral oil (positive control) was applied topically to the clipped interscapular region twice weekly. A second negative control group went untreated. Application continued for 80 weeks or until a neoplasm was clinically diagnosed as an "advanced tumor". During the study, animals were observed twice daily for signs of toxicity. A skin lesion that persisted for at least one week and grew to the size of approximately 1 mm, was classified as a papilloma. If the lesion grew and invaded surrounding tissue and became ulcerated and necrotic, it was diagnosed as an "advanced tumor". The skin was examined histologically for non-neoplastic and neoplastic lesions. Histological examination was performed on the organs of all animals at the conclusion of the study.
NOAEL (NOEL)	50 mg
Actual Dose Received by Dose Level and Sex Toxic Response/effects by Dose Level	50 mg Three of 50 mice treated with heptanoic acid developed benign skin tumors with a latent period of 65.7 weeks. Skin tumors were recorded for 45 of the 50 mice treated with 0.05% benzo(a)pyrene in mineral oil. One squamous cell carcinoma was reported in the untreated control group and no skin tumors were reported in the mineral oil group. The incidence of lesions in organs (e.g., hepatocarcinomas) of the negative control groups and test group were similar. Histologically the test group exhibited a slightly higher incidence of fibrosis and pigmentation of the skin.
Conclusion Remarks	Heptanoic acid (50 mg) administered to the skin of male mice twice weekly for 80 weeks did not show any evidence of carcinogenicity to the skin or other organs.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Suskind R. (1985) Chronic mouse dermal toxicity study. Kettering Laboratory. Unpublished report.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	28-day dermal toxicity study

GLP	No
Year	1981
Species/strain	Rabbit/New Zealand White
Sex	Male and Female
Route of Administration	Dermal
Doses/concentration Levels	500 mg/kg/day
Exposure Period	Five days per week for two weeks
Frequency of Treatment	Daily
Control Group	Mineral
Post Exposure Observation Period	14 days
Remarks for Test Conditions	A single dose of 500 mg/kg of heptanal in mineral oil (25% solution) was applied to the freshly clipped lateral and dorsal areas of groups of rabbits (5/sex/group) daily for 5 days per week for 2 weeks. The skin of half the animals was abraded prior to the first, sixth, and eighth dose. A control group was treated with mineral oil only. Viability was recorded twice daily, observations for skin irritation were made daily, and body weights were measured weekly. After 2 weeks 6 animals (3 with abraided and 3 with intact skin) were necropsied with the remaining 4 animals sacrificed after an additional 2-week recovery period. Tissues from 29 organs were removed and preserved in 10% formalin.
NOAEL (NOEL)	<500 mg/kg/day
Actual Dose Received by Dose Level and Sex	500 mg/kg/day
Toxic Response/effects by Dose Level	No mortalities were observed at weeks 2 and 4. Most animals exhibited a weight loss after one or two weeks, but animals held for an additional two-week recovery period exhibited normal weight gain compared to controls. Most animals showed local dermal irritation reflected by slight to moderate erythema during the first week. Localized necrosis and exfoliation occurred in most animals during the second week. Microscopic evaluation revealed epidermal necrosis, epidermal hyperplasia, and hyperkeratosis at the application site. The skin application sites of animals held to week 4 appeared healed. The sites were re-epithelialized and continuous with normal follicular structure and population. No other microscopic alterations were reported for any other tissue that could be related to administration of the test material.
Statistical evaluations?	None
Conclusion Remarks	A single dose of 500 mg/kg of heptanal applied daily to the abraided and intact skin of rabbits 5 days per week for 2 weeks, resulted in site-specific irritation effects that were healed after a 2 week recovery period.

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The only temporary effect, localized irritation involving necrosis, hyperkeratosis and exfoliation, healed in the 2-week post-treatment period.
References	Auletta C. (1981) A 28-day toxicity study in rabbits. Project No.6510-80. Unpublished report to FFHPVC.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	28-day dermal toxicity study
GLP	No
Year	1981
Species/strain	Rabbit/New Zealand White
Sex	Male and Female
Route of Administration	Dermal
Doses/concentration Levels	500 mg/kg/day
Exposure Period	Five days per week for two weeks
Frequency of Treatment	Daily
Control Group	Mineral
Post Exposure Observation Period	14 days
Remarks for Test Conditions	A single dose of 500 mg/kg of nonanal in mineral oil (25% solution) was applied to the freshly clipped lateral and dorsal areas of groups of rabbits (5/sex/group) daily for 5 days per week for 2 weeks. The skin of half the animals was abraded prior to the first, sixth, and eighth dose. A control group was treated with mineral oil only. Viability was recorded twice daily, observations for skin irritation were made daily, and body weights were measured weekly. After 2 weeks 6 animals (3 with abraided and 3 with intact skin) were necropsied with the remaining 4 animals sacrificed after an additional 2-week recovery period. Tissues from 29 organs were removed and preserved in 10% formalin.
NOAEL (NOEL)	<500 mg/kg/day
Actual Dose Received by Dose Level and Sex	500 mg/kg/day
Toxic Response/effects by Dose Level	No mortalities were observed at weeks 2 and 4. Several animals exhibited decreased food consumption during weeks 2 and 3. Most animals exhibited a weight loss after one or two weeks, but animals held for an additional two-week recovery period exhibited normal weight gain compared to controls. Most animals showed local dermal irritation reflected by slight to moderate erythema during the first week. Localized necrosis

Statistical evaluations?	and exfoliation occurred in most animals during the second week. Microscopic evaluation revealed epidermal necrosis, epidermal hyperplasia, and hyperkeratosis at the application site. The skin application sites of animals held to week 4 appeared healed. The sites were re-epithelialized and continuous with normal follicular structure and population. No other microscopic alterations were reported for any other tissue that could be related to administration of the test material.
Conclusion Remarks	None
Conclusion Remarks	A single dose of 500 mg/kg of nonanal applied daily to the abraded and intact skin of rabbits 5 days per week for 2 weeks, resulted in site-specific irritation effects that were healed after a 2 week recovery period.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The only temporary effect, localized irritation involving necrosis, hyperkeratosis and exfoliation, healed in the 2-week post-treatment period.
References	Auletta C. (1981) A 28-day toxicity study in rabbits. Project No.6510-80. Unpublished report to FFHPVC.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	28-day dermal toxicity study
GLP	No
Year	1981
Species/strain	Rabbit/New Zealand White
Sex	Male and Female
Route of Administration	Dermal
Doses/concentration Levels	500 mg/kg/day
Exposure Period	Five days per week for two weeks
Frequency of Treatment	Daily
Control Group	Mineral
Post Exposure Observation Period	14 days
Remarks for Test Conditions	A single dose of 500 mg/kg of heptanoic acid in mineral oil (25% solution) was applied to the freshly clipped lateral and dorsal areas of groups of rabbits (5/sex/group) daily for 5 days per week for 2 weeks. The skin of half the animals was abraded prior to the first, sixth, and eighth dose. A control group was treated with mineral oil only. Viability was recorded twice daily, observations for skin irritation were made daily, and body weights were measured weekly. After 2 weeks 6 animals (3 with abraded and 3 with intact skin) were necropsied with the

NOAEL (NOEL)	remaining 4 animals sacrificed after an additional 2-week recovery period. Tissues from 29 organs were removed and preserved in 10% formalin. <500 mg/kg/day
Actual Dose Received by Dose Level and Sex	500 mg/kg/day
Toxic Response/effects by Dose Level	One mortality was recorded at day 11. Most animals exhibited a weight loss after two weeks, but animals held for an additional two-week recovery period exhibited normal weight gain compared to controls. All animals showed localized severe erythema, slight to severe edema, necrosis, desquamation and exfoliation by the second week of treatment. Some animals showed evidence of ocular irritation. Some animals showed decreased food consumption during the first 3 weeks of the study. All animals were free of signs of dermal and systemic toxicity at the end of the 2-week recovery period. Microscopic evaluation revealed epidermal necrosis, epidermal hyperplasia, and hyperkeratosis at the application site. The skin application sites of animals held to week 4 appeared healed. The sites were re-epithelialized and continuous with normal follicular structure and population. No other microscopic alterations were reported for any other tissue that could be related to administration of the test material.
Statistical evaluations?	None
Conclusion Remarks	A single dose of 500 mg/kg of heptanoic acid applied daily to the abraded and intact skin of rabbits 5 days per week for 2 weeks, resulted in site-specific irritation effects that were healed after a 2 week recovery period.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The only temporary effect, localized irritation involving necrosis, hyperkeratosis and exfoliation, healed in the 2-week post-treatment period.
References	Auletta C. (1981) A 28-day toxicity study in rabbits. Project No.6510-80. Unpublished report to FFHPVC.

Substance Name	Nonanal (data for metabolite, nonanoic acid)
CAS No.	124-19-6
Method/guideline	28-day dermal toxicity study
GLP	No
Year	1981
Species/strain	Rabbit/New Zealand White
Sex	Male and Female
Route of Administration	Dermal
Doses/concentration Levels	500 mg/kg/day

Exposure Period	Five days per week for two weeks
Frequency of Treatment	Daily
Control Group	Mineral
Post Exposure Observation Period	14 days
Remarks for Test Conditions	A single dose of 500 mg/kg of nonanoic acid in mineral oil (25% solution) was applied to the freshly clipped lateral and dorsal areas of groups of rabbits (5/sex/group) daily for 5 days per week for 2 weeks. The skin of half the animals was abraded prior to the first, sixth, and eighth dose. A control group was treated with mineral oil only. Viability was recorded twice daily, observations for skin irritation were made daily, and body weights were measured weekly. After 2 weeks 6 animals (3 with abraded and 3 with intact skin) were necropsied with the remaining 4 animals sacrificed after an additional 2-week recovery period. Tissues from 29 organs were removed and preserved in 10% formalin.
NOAEL (NOEL)	<500 mg/kg/day
Actual Dose Received by Dose Level and Sex	500 mg/kg/day
Toxic Response/effects by Dose Level	No mortalities were observed during the study. Most animals exhibited a weight loss after two weeks, but animals held for an additional two-week recovery period exhibited normal weight gain compared to controls. Most animals showed localized slight to severe erythema, slight to severe edema, necrosis, desquamation and exfoliation by the second week of treatment. Some animals showed evidence of ocular irritation. Some animals showed decreased food consumption during the weeks 2 and 3 of the study. All animals were free of signs of dermal and systemic toxicity at the end of the 2-week recovery period. Microscopic evaluation revealed epidermal necrosis, epidermal hyperplasia, and hyperkeratosis at the application site. The skin application sites of animals held to week 4 appeared healed. The sites were re-epithelialized and continuous with normal follicular structure and population. No other microscopic alterations were reported for any other tissue that could be related to administration of the test material.
Statistical evaluations?	None
Conclusion Remarks	A single dose of 500 mg/kg of nonanoic acid applied daily to the abraded and intact skin of rabbits 5 days per week for 2 weeks, resulted in site-specific irritation effects that were healed after a 2 week recovery period.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The only temporary effect, localized irritation involving necrosis, hyperkeratosis and exfoliation, healed in the 2-week post-treatment period.
References	Auletta C. (1981) A 28-day toxicity study in rabbits. Project No.6510-80. Unpublished report to FFHPVC.

4.5 Reproductive Toxicity

Substance Name	Heptanal (data for a structurally related aldehyde, 5-heptenal, 2,6-dimethyl)
CAS No.	111-71-7
Method/guideline	Virgin female Sprague-Dawley rats (10/group) were orally administered a vehicle or the test material at 3 dosages for one week prior to a 7-day cohabitation period through gestation, parturition and a 4-day postpartum period. Study duration was 39 days.
Test Type	Reproductive/Developmental study
GLP	GLP Regs. FDA (1987)
Year	1990
Species/Strain	Rat/Sprague-Dawley
Sex	Female/10/group
Route of Administration	Oral/gavage
Duration of Test	39 days
Doses/Concentration	0, 300, 1500 & 3000 mg/kg/day
Premating Exposure period for males	NG
Premating Exposure period for females	7 days
Frequency of Treatment	Daily
Control Group and Treatment	Corn Oil vehicle, 5 ml/kg/day
Remarks for Test Conditions	Mating, day 0 of gestation identified on basis of spermatozoa in vaginal smear. Viability was monitored twice daily during the study. Rats were observed daily for clinical signs approximately 30 minutes after gavage administration. Measurement of body weight was performed weekly. Food consumption measurement was also conducted weekly during the pre mating/pre mating period and then on days 0, 6, 14, 16, 21, and 25 of gestation and on days 1 and 4 of lactation/postparturition. Mating performance was evaluated daily during the cohabitation period. Dams were evaluated daily during gestation for duration of gestation, maternal behavior, litter size and pup viability. Dams that did not deliver litters were sacrificed on day 25 of presumed gestation and dams that did deliver litters were sacrificed on days 4 or 5 of lactation. All dams were examined for gross lesions and implantation sites. Ovaries from all dams and any observed gross lesions were preserved in neutral 10% formalin for possible evaluation. Vital signs at birth were determined for pups that were stillborn or died before the initial examination of the litter. Each litter was evaluated for viability a minimum of twice daily during the 4-day

	lactation period. Dead pups were removed and necropsied. Tissues with gross lesions were preserved for possible examination. Pups in each litter were counted and observed for nursing behavior and physical abnormalities daily. Pup body weights were measured on days 1 and 4 of postparturition.
NOAEL(NOEL)	300 mg/kg/d (maternal NOAEL)
LOAEL(LOEL)	1500 mg/kg/d (maternal)
Parental data and F1 as Appropriate	Clinical signs at 1500 and 3000 mg/kg in dams included decreased activity and excess salivation during the pre-gestation period and increased ($P<0.01$) salivation in the high dose group during gestation. Significant ($P<0.05$ to <0.01) decreases in body weight and absolute and relative food consumption were measured during the premating period. Eight rats of 10 in the high dose group were moribund or found dead on days 2, 3, and 4 of the premating period. Maternal body weights were decreased during gestation for the mid- and high-dose groups of dams. Decreased body weights and absolute and relative food consumption in the 300 mg/kg bw/day group occurred only during premating and were not considered adverse effects. One of the two surviving high-dose dams delivered a litter that died during the 4-day lactation period. Mating and fertility at the high dose were similar to controls. Measurements of mating success and fertility were similar for controls, low- and mid-dose groups.
Offspring Toxicity F1 and F2	Significant ($P<0.05$ to <0.01) decreases in pup viability occurred for middle and high dose groups as compared to controls. The mid-dose litters were significantly less ($P<0.05$) than control group litters. High-dose litters weighed remarkably less than controls. No changes in averages for duration of cohabitation or gestation, implantation sites or pup sex ratios were seen at any dose levels. No malformations or gross lesions in pups were attributable to the test material.
Statistical Evaluation	ANOVA followed by Dunnett's test
Remarks for Results	The decreased body weights and food consumption reported at 300 mg/kg bw/d during premating period were not considered adverse. Based on the significant decrease in ($P<0.05$) in pup weight at birth and pup viability in the mid-dose group, the NOAEL for the F1 offspring was reported to be >300 mg/kg bw/day but <1500 mg/kg bw/day.
Conclusion Remarks	Dose levels of 300 mg/kg bw/day of the test material (5-heptenal, 2,6-dimethyl) had no adverse effects on the reproductive performance of female Sprague-Dawley rats or the growth or development of their offspring.
Data Reliabilities Qualities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	Study met GLP Guidelines of U.S. Food and Drug Administration (1987) Good Laboratory Practice Guidelines; Final Rule. Fed. Reg. 9/4/87. Part VI, Vol. 52, No. 172. The study was published in a peer-reviewed journal, Teratology.
References	Vollmuth T.A., Bennett, M.B., Hoberman, A.M. and Christian, M.S. (1995) An Evaluation of Food Flavoring Ingredients Using an In Vivo Reproductive and Developmental Toxicity Screening Test. Teratology 41(5), 597.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Virgin female Sprague-Dawley rats (10/group) were orally administered a vehicle or the test material at 3 dosages for one week prior to a 7-day cohabitation period through gestation, parturition and a 4-day postpartum period. Study duration was 39 days
Test Type	Reproductive/Developmental Toxicity Study
GLP	GLP Regs. FDA (1987)
Year	1990
Species/Strain	Rat/Sprague-Dawley
Sex	Female/10/group
Route of Administration	Oral/gavage
Duration of Test	39 days
Doses/Concentration	0, 200, 1000 & 2000 mg/kg/day
Premating Exposure period for females	7 days
Frequency of Treatment	Daily
Control Group and Treatment	Corn Oil vehicle, 5 ml/kg/day
Remarks for Test Conditions	<p>Mating, day 0 of gestation identified on basis of spermatozoa in vaginal smear. Viability was monitored twice daily during the study. Rats were observed daily for clinical signs approximately 30 minutes after gavage administration. Measurement of body weight was performed weekly. Food consumption measurement was also conducted weekly during the premating/premating period and then on days 0,6,14,16,21, and 25 of gestation and on days 1 and 4 of lactation/postparturition. Mating performance was evaluated daily during the cohabitation period. Dams were evaluated daily during gestation for duration of gestation, maternal behavior, litter size and pup viability. Dams that did not deliver litters were sacrificed on day 25 of presumed gestation and dams that did deliver litters were sacrificed on days 4 or 5 of lactation. All dams were examined for gross lesions and implantation sites. Ovaries from all dams and any observed gross lesions were preserved in neutral 10% formalin for possible evaluation. Vital signs at birth were determined for pups that were stillborn or died before the initial examination of the litter. Each litter was evaluated for viability a minimum of twice daily during the 4-day lactation period. Dead pups were removed and necropsied. Tissues with gross lesions were preserved for possible examination. Pups in each litter were counted and observed for nursing behavior and physical abnormalities daily. Pup body</p>

	weights were measured on days 1 and 4 of postparturition.
NOAEL(NOEL)	<200 mg/kg/d (maternal NOAEL)
LOAEL(LOEL)	>1000 mg/kg/d (maternal)
Parental data and F1 as Appropriate	One and 3 deaths were reported in the 1000 and 2000 mg/kg bw/day dose groups, respectively. Clinical signs at 200 mg/kg bw/day in dams during premating and gestation included a significant increase in rales ($P<0.01$). This effect was not reported during the lactation period. In the 1000 and 2000 mg/kg bw/day dose group, significant increases in the incidence of rales ($P<0.01$), excess salivation ($P<0.01$) was reported during premating and gestation. Excess salivation continued during lactation in the high-dose group. Other significant ($P<0.01$) effects during gestation in the high-dose group included decreased activity, ungroomed coat and labored breathing. The 2000 mg/kg bw/day group showed reduced body weight gains during premating, and significantly ($P<0.05$ to <0.01) decreased average maternal body weights on days 10 and 16 of gestation. Average and relative food consumption was reduced in the high-dose group of dams throughout the study. The high dose also was associated with reduced mating and fertility that were related to mortality. The duration of cohabitation and fertility and gestation indices 200, 1000, or 2000 mg/kg bw/day were not different from comparable indices in three control group.
Offspring Toxicity F1 and F2	The high-dose group exhibited reduced pup weights on day 4 postparturition. No biologically relevant or statistically significant differences in the number of implantations, duration of gestation, the percentage of dams delivering one or more live pups, and the pup viability index were observed. No malformations or gross lesions were observed in pups at any dose levels.
Statistical Evaluation	ANOVA followed by Dunnett's test
Remarks for Results	Based on the significant ($P<0.01$) increase of rales in the low-dose group of dams reported during premating and gestation period, the NOAEL for dams was <200 mg/kg bw/day. Based on reduced pup body weight on day 4 postpartum at the high dose, the NOAEL for the offspring was >1000 mg/kg bw/day and <2000 mg/kg bw/day.
Conclusion Remarks	Dose levels of 200 mg/kg bw/day of heptanoic acid had no significant adverse effects on the reproductive performance of female Sprague-Dawley rats or the growth or development of their offspring.
Data Reliabilities Qualities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	Study met GLP Guidelines of U.S. Food and Drug Administration (1987) Good Laboratory Practice Guidelines; Final Rule. Fed. Reg. 9/4/87. Part VI, Vol. 52, No. 172. The study was published in a peer-reviewed journal, Teratology.
References	Vollmuth T.A., Bennett, M.B., Hoberman, A.M. and Christian, M.S. (1995) An Evaluation of Food Flavoring Ingredients Using an In Vivo Reproductive and Developmental Toxicity Screening Test. Teratology 41(5): 597.

Substance Name	Heptanal
CAS No.	111-71-7
Test Type	Reproduction Study
GLP	No
Year	1941
Species/Strain	Rat/Wistar female, piebald
Sex	Female
Route of Administration	Oral (gavage)
Duration of Test	20 day
Doses/Concentration	0.50 ml/150-200 g female rat/day or 2050 mg/kg bw/day
Premating Exposure period for females	None reported
Frequency of Treatment	Daily
Control Group and Treatment	No control group
Remarks for Test Conditions	Several young female rats were mated with one male and the mating success was monitored by daily vaginal smears. Ten females were used in the study. Female rats were maintained on Purina Dog Chow and water ad libitum. Body weights were measured daily and the difference in weight between the weight on the day of insemination and immediately after parturition were also recorded. There was no reported of resorptions in any of the 10 female rats.
NOAEL(NOEL)	2050 mg/kg bw/day
Statistical Evaluation	None
Conclusion Remarks	Oral administration of 2050 mg/kg bw/day of heptanal resulted in no evidence of reproductive toxicity in female Wistar rats.
Data Reliabilities Qualities	Reliability code 3. Not reliable. Study contained measurement of limited number of parameters measuring reproduction.
Remarks for Data Reliability	Oral study was a preliminary study in Wistar rats. The results of the study were used to design a second study using the intraperitoneal route of administration. In the second study heptanal did not impair the reproductive system of rats.
References	Carruthers C. and Stowall R.E. (1941) Influence of heptaldehyde on the pregnancy in rats. Cancer Research, 1(9):724-728.

4.6 Developmental/Teratogenicity Toxicity

Substance Name	Octanal (data for a metabolite, octanoic acid)
CAS No.	124-13-0
Method/guideline	Chernoff/Kalock assay
Test Type	Developmental toxicity
GLP	NG
Year	1994
Species/strain	Sprague-Dawley rat
Sex	Female
Route of Administration	Gavage
Duration of Test	28 days
Doses/concentration Levels	0, 1125, 1500 mg/kg/day
Exposure Period	10 days
Frequency of Treatment	Once daily (days 6-15 of gestation)
Control Group and Treatment	Controls used but were not defined.
Remarks for Test Conditions	High dose level expected to produce moderate maternal toxicity and the low dose was 75% of the high dose
LOAEL (LOEL) Maternal Toxicity	1125 mg/kg bw/d
NOAEL (NOEL) Developmental Toxicity	1125 mg/kg bw/d
Maternal Data with Dose Level	No effect on # of implants, but decreased body weight in dams at both dose levels.
Fetal Data with Dose Level	Significant decrease ($p < 0.05$) in the number of live pups at the high dose only; no effect on perinatal loss (%) or pup weight at either dose.
Statistical Evaluation	Yes
Conclusion Remarks	Octanoic acid induced a significant decrease in the number of live pups in Sprague-Dawley rats but only at a dose, which causes maternal toxicity.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions. Study on development toxicity potential of a variety of organic acids. No visceral or skeletal examinations were performed.
Remarks for Data Reliability	Adequate number of animals, statistics, concentrations tested; but a limited discussion of data.
References	Narotsky, M.G., E.Z. Francis and R.J. Kavlock (1994) Developmental toxicity and structure-activity relationships of aliphatic acids including dose-response assessment of valproic

acid in mice and rats. Fundamental and Applied Toxicology
22:251-265.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Embryo/fetal and teratogenesis
Test Type	Embryo-fetotoxicity
GLP	NG
Year	1983
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
Route of Administration	Gavage
Duration of Test	20 days
Doses/concentration Levels	1000 mg/kg bw/day
Exposure Period	9 days (days 6-15 of gestation)
Frequency of Treatment	One daily (day 6-15)
Control Group and Treatment	Vehicle (Corn oil) only
Remarks for Test Conditions	Groups of male (1) and female (2) rats were bred until mating was confirmed. Following mating, a group of 22 female rats were given 1000 mg/kg of heptanoic acid daily for days 6 to 15 of pregnancy. Body weights and food consumption were measured regularly during gestation. On day 20 of gestation, females were sacrificed and the number of corpora lutea/ovary, implantation sites, early and late resorptions, and live and dead fetuses were recorded. One third of the fetuses received visceral examinations and two-thirds were subjected to skeletal examination. Dam uterine weights were measured and tissues from ovaries and uterus were preserved for microscopic examination. All data was subjected to ANOVA analysis (Dunnett's T-test)
NOAEL (NOEL) maternal toxicity	1000 mg/kg bw/day
NOAEL (NOEL) developmental toxicity	1000 mg/kg bw/day
Maternal data with dose level	Based on lack of mortality and clinical observations, no significant difference between body weight changes and food and water consumption for test and control animals, and the lack of any gross pathology, it was concluded that there was no maternal toxicity observed in this study.
Fetal Data with Dose Level	Based on mean ovarian, uterine, litter size, pregnancy rates, corpora lutea, implantation sites and efficiency, fetal viability, fetal size and sex, uterine weights, gross pathology, and

Statistical Evaluation	visceral and skeletal examinations, there was no significant difference between the test and control group. ANOVA (Dunnett's T-test)
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Conclusion remarks	There was no evidence of embryo toxicity, fetal toxicity, or teratogenesis when pregnant female rats were given 1000 mg/kg bw/day of heptanoic acid on days 6-15 of pregnancy.
References	Serota D.G. (1983) Evaluation of the embryo/fetal toxicity and teratogenic effects of a series of ten compounds in pregnant Sprague-Dawley rats. Project No 299-534. Unpublished Report to FFHPVC.

Substance Name	Nonanal (data for a metabolite, nonanoic acid)
CAS No.	124-19-6
Method/guideline	Embryo/fetal and teratogenesis
Test Type	Embryo-fetotoxicity
GLP	NG
Year	1983
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
Route of Administration	Gavage
Duration of Test	20 days
Doses/concentration Levels	1500 mg/kg bw/day
Exposure Period	9 days (days 6-15 of gestation)
Frequency of Treatment	One daily (day 6-15)
Control Group and Treatment	Vehicle (Corn oil) only
Remarks for Test Conditions	Groups of male (1) and female (2) rats were bred until mating was confirmed. Following mating, a group of 22 female rats were given 1000 mg/kg of nonanoic acid daily for days 6 to 15 of pregnancy. Body weights and food consumption were measured regularly during gestation. On day 20 of gestation, females were sacrificed and the number of corpora lutea/ovary, implantation sites, early and late resorptions, and live and dead fetuses were recorded. One third of the fetuses received visceral examinations and two-thirds were subjected to skeletal examination. Dam uterine weights were measured and tissues from ovaries and uterus were preserved for microscopic examination. All data was subjected to ANOVA analysis (Dunnett's T-test).
NOAEL (NOEL) maternal toxicity	1500 mg/kg bw/day

NOAEL (NOEL) developmental toxicity	1500 mg/kg bw/day
Maternal data with dose level	Based on lack of mortality and clinical observations, no significant difference between body weight changes and food and water consumption for test and control animals, and the lack of any gross pathology, it was concluded that there was no maternal toxicity observed in this study.
Fetal Data with Dose Level	Based on mean ovarian, uterine, litter size, pregnancy rates, corpora lutea, implantation sites and efficiency, fetal viability, fetal size and sex, uterine weights, gross pathology, and visceral and skeletal examinations there were no significant difference between the test and control group.
Statistical Evaluation	ANOVA (Dunnett's T-test)
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Conclusion remarks	There was no evidence of embryo toxicity, fetal toxicity, or teratogenesis when pregnant female rats were given 1500 mg/kg bw/day of nonanoic acid on days 6-15 of pregnancy.
References	Serota D.G. (1983) Evaluation of the embryo/fetal toxicity and teratogenic effects of a series of ten compounds in pregnant Sprague-Dawley rats. Project No 299-534. Unpublished report to FFHPVC.

Substance Name	Heptanoic acid (data on homologue octanoic acid)
CAS No.	111-14-8
Test Type	Developmental Toxicity
GLP	NG
Year	1994
Species/strain	Sprague-Dawley rat
Sex	Female
Route of Administration	Oral (gavage)
Duration of Test	20 day of gestation
Doses/concentration Levels	18.75 mmol/kg (2700 mg/kg)
Exposure Period	One day
Frequency of Treatment	Single dose on day 20 of gestation
Control Group and Treatment	Controls received no test substance, not specified
Remarks for Test Conditions	All agents were administered undiluted by oral gavage on the morning of day 12 of rat gestation (day 0 = morning of finding vaginal plug). On day 20 of gestation, rats were killed by chloroform overdose, and survivability, # of implantation sites, and mean fetal weight were recorded.
NOAEL (NOEL) maternal toxicity	18.75 mmol/kg (2700 mg/kg)

Maternal data with dose level	Maternal toxicity considered severe at this dose level.
Fetal Data with Dose Level	Octanoic acid devoid of embryotoxic effects except for a slight reduction of fetal weight may be attributable to the severe maternal toxicity observed at the 2700 mg/kg dose.
Statistical Evaluation	None described
Data Qualities Reliabilities	Reliability code 3. Not reliable. Study was experimental in nature. Contained a limited number of measurements on development.
Remarks for Data Reliability	Lacking full description of controls and statistics.
Conclusion remarks	Octanoic acid was not embryotoxic in this assay.
References	Scott, Jr., W.J., M.D. Collins and H. Nau (1994) Pharmacokinetic determinants of embryotoxicity in rats associated with organic acids. Env. Health Perspectives, 102 (Suppl. 11) 97-101.

Substance Name	Octanal (data for metabolite of octanoic acid)
CAS No.	124-13-0
Method/guideline	Teratogenesis
Test Type	Developmental toxicity
GLP	NG
Year	1986
Species/strain	NMRI mice
Sex	Female
Route of Administration	Subcutaneous injection
Duration of Test	10 days
Doses/concentration Levels	0, 600 mg/kg body weight
Exposure Period	Single injection on day 8 of gestation
Frequency of Treatment	One
Control Group and Treatment	Control given water vehicle sc only.
Remarks for Test Conditions	Groups of 15 mice were treated on day 8. Examinations were performed on day 18 of gestation. Implantation sites were counted and each live fetus was individually weighed and inspected for the presence of neural tube defects.
Fetal Data with Dose Level	15% embryoletality (7% in controls); No effect on fetal weigh or on percentage of exencephaly in live fetuses.
Statistical Evaluation	Yes
Data Qualities Reliabilities	Reliability code 3. Not reliable. Experimental study in which a single dose was administered on day 8 of gestation. Fetal

examination was limited to analysis of neural tube defects.

Remarks for Data Reliability The study included an adequate number of animals, statistics, and concentrations tested, but a limited description of data. Published in a peer-reviewed journal.

References Nau, H. and W. Loscher (1986) Pharmacologic evaluation of various metabolites and analogs of valproic acid: Teratogenic potencies in mice. Fund. Appl. Toxicol. 6:669-676.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Teratogenesis
Test Type	Frog embryo teratogenesis assay
GLP	NG
Year	1996
Species/strain	Xenopus embryos
Sex	Not reported
Route of Administration	In solution
Duration of Test	96 hrs
Doses/concentration Levels	8 concentrations (not specified) and 1 control
Exposure Period	96 hrs
Frequency of Treatment	Single exposure
Control Group and Treatment	Controls used but were not defined.
Remarks for Test Conditions	Embryos were collected following hormone-induced breed. Each group of 25 embryos was exposed to one of 8 concentrations of acid and a control, each acid was tested three times and data were pooled to calculate 96 hrs LC50 (lethality) and 96 hrs EC50 (malformation) and development hazard index (DHI).
Fetal Data with Dose Level	LC50 = 319.6 (313-324) mg/l; EC50 = 51.3 (48-55) mg/l; DHI = 6.2
Statistical Evaluation	Yes
Conclusion Remarks	Developmental hazard index was found to be greater than 5 indicating a moderate hazard according to the authors.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Study was published in a peer-reviewed journal.
References	Dawson, D.A., W. Schultz and R.S. Hunter (1996) Developmental toxicity of carboxylic acids to Xenopus embryos: A quantitative structure-activity relationship and computer-automated structure evaluation. Teratogenesis, Carcinogenesis

and Mutagenesis 16:109-124.

Substance Name	Heptanoic acid (data for homologue octanoic acid)
CAS No.	124-07-2
Method/guideline	Teratogenesis
Test Type	Frog embryo teratogenesis assay
GLP	NG
Year	1996
Species/strain	Xenopus embryos
Sex	Not reported
Route of Administration	In solution
Duration of Test	96 hrs
Doses/concentration Levels	8 concentrations (not specified) and 1 control
Exposure Period	96 hrs
Frequency of Treatment	Single exposure
Control Group and Treatment	Controls used but were not defined.
Remarks for Test Conditions	Embryos were collected following hormone-induced breed, each group of 25 embryo was exposed to one of 8 concentrations of acid and a control, each acid was tested three times and data were pooled to calculate 96h LC50 (lethality) and 96h EC50 (malformation) and development hazard index (DHI).
Fetal Data with Dose Level	LC50 = 127.1 (119-136) mg/l; EC50 = 28.1 (26-30) mg/l; DHI = 4.5
Statistical Evaluation	Yes
Conclusion Remarks	Developmental hazard index was found to be less than 5 indicating a low hazard according to the authors.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Study was published in a peer-reviewed journal.
References	Dawson D.A., W. Schultz and R.S. Hunter (1996) Developmental toxicity of carboxylic acids to xenopus embryos: a quantitative structure-activity relationship and computer-automated structure evaluation. Teratogenesis, Carcinogenesis and Mutagenesis 16:109-124.

Substance Name	Nonanal (data for metabolite of nonanal, nonanoic acid)
CAS No.	124-19-6
Method/guideline	Teratogenesis
Test Type	Frog embryo teratogenesis assay
GLP	NG
Year	1996
Species/strain	Xenopus embryos
Sex	Not reported
Route of Administration	In solution
Duration of Test	96 hrs
Doses/concentration Levels	8 concentrations (not specified) and 1 control
Exposure Period	96 hrs
Frequency of Treatment	Single exposure
Control Group and Treatment	Controls used but were not defined.
Remarks for Test Conditions	Embryos were collected following hormone-induced breed, each group of 25 embryo exposed to one of 8 concentrations of acid and a control, each acid was tested three times and data were pooled to calculate 96 hrs LC50 (lethality) and 96 hrs EC50 (malformation) and development hazard index (DHI). LC50 = 32.7 (29-36) mg/l; EC50 = 6.5 (6-7) mg/l; DHI = 5.0
Fetal Data with Dose Level	LC50 = 32.7 (29-36) mg/l; EC50 = 6.5 (6-7) mg/l; DHI = 5.0
Statistical Evaluation	Yes
Conclusion Remarks	DHI was found to be 5 indicating a low to moderate hazard according to the authors
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Study was published in a peer-reviewed journal.
References	Dawson D.A., W. Schultz and R.S. Hunter (1996) Developmental toxicity of carboxylic acids to xenopus embryos: a quantitative structure-activity relationship and computer-automated structure evaluation. Teratogenesis, Carcinogenesis and Mutagenesis 16:109-124.